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QUASI-REGULAR IMPURITY DISTRIBUTION DRIVEN BY CHARGE-DENSITY WAVE

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ABSTRACT

The displacive motion of the impurity distribution immersed into the one–dimensional system has recently been studied in detail as one kind of quasi–regularity driven by CDW. As a further investigation of this problem we develop here a microscopical model for a different kind of quasi–regular impurity distribution driven by CDW, consisting of the modulation in the probability of occupied sites. The dependence on impurity concentration and temperature of relevant CDW quantities is obtained. Data reported in the quasi–1D materials $NbSe_3$ and Ta_2NiSe_7 (particularly, thermal hysteresis effects at CDW transition) are interpreted in the framework of the present model. Possible similarities to other physical systems are also suggested.

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1 INTRODUCTION

The charge – density – wave (C D W) state is a form of two – fermion condensate consisting of a coherent superposition of electron – hole pairs having a given value, Q, of the total momentum. In the one – dimensional (1D) system, to which we restrict ourselves in this work, this value is twice the Fermi value reduced to the first Brillouin zone ($Q = 2k_F \ mod \ G$, G — basic wave vector of reciprocal lattice). Let us now assume that we add impurities to this system. They will be supposed to be ordinary (non – magnetic) and to have no internal degree of freedom. The electrons will then scatter on them. By assuming furthermore that the spatial distribution of impurities in the chains is perfectly random, the scattering processes will be incoherent, yielding thereby the break – up of coherent superposition of electron – hole pairs in the CDW condensate. Actually, the assumption of perfect randomness of impurity distribution was made in most of studies dealing with this problem (see, *e.g.* [1 – 4] for recent reviews). Moreover, it was assumed that the spatial distribution of impurities is the same in the normal state and in the CDW one. Such an impurity distribution may be termed perfectly random and rigid [5]. Its destructive effect, as mentioned above, has been studies by means of a multitude of methods [6-10].

However, very simple electrostatic arguments can be invoked to show that — unlike in the normal state — the perfectly random and rigid impurity distribution does not correspond to the most stable state of the system in the CDW state. Once the static modulation of electron density (i.e. the CDW) and the accompanying Peierls distortion of lattice are installed into the system, impurities will tend to adjust their positions such that to minimize the energy of their interaction with lattice and electrons. Consequently, a quasi – regularity in their spatial distribution having the same wave vector Q is expected. In a series of papers [11 – 13, 5], the occurrence of a CDW – driven displacive motion of impurity distribution has been discussed. It has been argued that this kind of Q – quasi regularity, having a similar form to the

Peierls lattice distortion itself, could be expected in the case of low mobility impurities. Non - trivial effects could be brought about by this displacive motion: reentrant CDW at the increase of impurity concentration, x, thermal hysteresis effects and a sensible broadening of the range of x – values compatible to a gapless CDW state [5].

However, this does not represent the most favoured state for the energetics of the CDW — impurity system. Most favorable would be that impurities could occupy those sites in the chain where they would take the maximum advantage from the presence of the CDW. This would correspond to a modulation in the probability (or, alternatively, concentration) of occupied sites by impurities.

One should argue that this modulation could effectively occurs in two realistic cases. Firstly, this could happen in the case where impurities could migrate through the crystal, via atomic diffusion processes, towards those sites where the energy of their interaction with the CDW is minimum. Experimental data reported for deuterated thiourea [13], blue bronze [14] and (cf. the presently proposed interpretation, Section 5) niobium triselenide [15] could be invoked in favour of such a modulation allowed for highly mobile impurities. Secondly, one may expect such a modulation in the distribution of impurities in connection with the manner in which a certain doped quasi - 1D material is synthezised. If this preparation process yields a material whose stable state is a CDW one, one would expect that, in the case where the process is slow enough, impurities would have the possibility to drift towards those sites at which the minimization of the total energy occurs; thence, a Q - modulation in the occupation probability. We argue that this is the case of the Krogmann salt (KCP) which possesses a Peierls – CDW distortion whatever the value of temperature where this quasi – 1D compound is stable; the microscopical description based on this assumption turned out to be successful in explaining a variety of experimental data reported for KCP [16, 17].

As stated previously [5], this CDW – driven quasi – regularity of impurity distri-

bution has to be accounted for besides the usual pair – breaking effect of impurities on the CDW condensate. The purpose of the present paper is to investigate this interplay between disorder and $2k_F$ – quasi - regularity associated with the impurity distribution in the 1D – CDW system for the second type of regularity described above. This study is intended to be complimentary to that done previously for the case of the CDW – driven displacive motion of impurity distribution [5]. Both aims and methods we shall use here are borrowed from the afore – mentioned investigation. Therefore, whenever possible, in order to avoid any repetition we shall skip irrelevant details and present only those calculations which render this paper self – contained.

The remaining part of this paper is organized in the following manner. The precise statement of the modulated impurity distribution is made in Section 2, where the description of the method of solution is also given. Two limiting models of the modulated impurity distributions are discussed in Sections 3 and 4; there, the dependence on impurity concentration and temperature of the relevant CDW quantities is derived in both cases. The last part of the paper, Section 5, is particularly devoted to the discussion of the experimental data reported in various quasi 1D CDW materials with impurities in the light of the results obtained within the present model.

2. COEXISTING CDW AND MODULATED IMPURITY DISTRIBUTION

It is well known that the electron – lattice interaction causes the (Peierls) distortion of the 1D periodic lattice [18],

$$\delta X_n = A_L \cos(QX_n + \varphi_L), \tag{1}$$

and the static modulation of the electron density (*i. e.* CDW),

$$\delta\rho(x) = \rho(x) - \rho_0 = \rho_1 \cos(Qx + \varphi). \tag{2}$$

Here $X_n = nd$ (d – interatomic spacing) denotes the sites occupied by the N atoms (ions) of the chain ($L = Nd$, L – length of the system), A_L and ρ_1 stand for the amplitudes of the $2k_F$ static distortions characterizing the Peierls – CDW state and the wave vector Q (defined in Introduction) is supposed to be incommensurate with respect to the underlined lattice periodicity; the remaining notations are obvious. In the clean system the quantities A_L and ρ_1 are proportional and could be taken as the CDW order parameter.

Let us now assume that N_i out of the N atoms of the lattice are replaced by impurities which could occupy (with various probabilites) the sites $\{Y_\nu\}$,

$$Y_\nu = X_{\overline{n}}, \tag{3}$$

in the lattice ($1 \leq \overline{n} \leq N$, $1 \leq \nu \leq N_i$). [3]

As discussed in Introduction, a modulation in the probability of sites occupied by impurities is expected in the case where they could reach the positions where the total energy of the system is minimum. In view of the overall $2k_F$ periodicity of the Peierls – CDW state, the most natural assumption to be made on this probability, $w(Y)$, is that it also possesses a $2k_F$ modulation:

$$w(Y) = \frac{1}{N}\sum_{n=1}^{N}[1 + w_1\cos(QY + \varphi_i)]\delta(Y - X_n). \tag{4}$$

Here w_1 is the amplitude of the fractional modulation probability, φ_i is a phase factor and the prefactor ensures the normalization

$$\int_0^L w(Y)dY = 1.$$

The presence of the Dirac – delta function in Equation (4) is the direct consequence of the type we have chosen for the impurity distribution, Equation (3). For the moment, we can think that Equation (4) is an Ansatz for the present problem whose form is justified by the qualitative arguments presented above. Later on we

[3] This choice, which corresponds to the case of substitutional impurities, is made only for simplicity; calculations could be done also for $Y_\nu = X_{\overline{n}} + const$ or for a continuous distribution ($0 \leq Y_\nu \leq L$).

shall return to this point in more detail (cf . Section 5). However, one should remark here that Equation (4) implicitly assumes a small probability of finding two impurity atoms (ions) in the same position (or, more realistically, very close), corresponding to the minimum energy. Nevertheless, this does not impose a severe low dilute limit. It only implies an average inter – impurity spacing much larger than the CDW wave length; in realistic situations [1 – 4], the latest only extends over several unit cells. In this way, Equation (4) plays a basic rôle in the present approach: it incorporates both the regularity (via the non-vanishing value of w_1) and the disorder (via the distribution function $w(Y)$ itself) related to the modulated impurity distribution we are going to study[4].

As the presence of impurities is essential, a precise statement of the framework adoted in the present investigation should be in order. It has been pointed out [20 – 21] that no long range order could exist in the presence of disorder in space dimensions less than four; impurities smear out the CDW transition. Practically this means that CDW ordering occurs in finite domains of the order of the correlation length. Insofar as the latest extends over many unit cells[5], one can argue that treating impurity effects on the static CDW properties by employing the methods used for infinite system is acceptable as a first – step investigation. [6] On the other hand, as usual in this kind of studies, we shall keep the picture of extended electronic states and ignore localization effects.

As always in problems involving impurities, one has to perform averaging over their spatial configuration at a certain step of calculations. As a rule, we shall take averages over impurities by means of the distribution function given by Equation (4) in the lowest non – vanishing order. This will allow us to keep (but also to separate

[4] The term *modulated impurity distribution*, we use here, was put forward in connection with the quasi – 1D compound KCP [16, 17]; simultaneously but independently a somewhat similar physical situation in deuterated thiourea has also been discussed and termed *defect density wave*[19].

[5] We mention in this context that the content of impurities in KCP ($K_2[Pt(CN)_4]Br_{0.3} \times 3.2H_2O$) is 0.3 bromine anions and 0.2 (extra) water molecules per formula unit;despite this large impurity content the correlation length exceeds 100 unit cells [17].

[6] Actually, this restriction is less severe in the present case; one would expect an enhancement in the correlation length by allowing a quasi – regularity of impurity distribution, Equation (4), as compared to the case of perfect randomness.

between) the coherent and incoherent effects brought about by impurities.

Following the lines of Ref. 5, we can get the total Hamiltonian, H, of the electron – lattice – impurity system. It consists of three parts

$$H \equiv H^0 + H_{scatt} + E_{elastic}. \tag{5}$$

The first part is diagonal(izable), the second corresponds to the incoherent electron-impurity scattering and the third represents the elastic energy. The first term has the form

$$H^0 \equiv H_0 + H_{coherent} = \sum_p \hat{\psi}_p^\dagger \, v_F \, p \, \hat{\sigma}_3 \, \hat{\psi}_p + \sum_p \hat{\psi}_p^\dagger (\Delta \hat{\sigma}_+ + \Delta^* \hat{\sigma}_-) \, \hat{\psi}_p, \tag{6}$$

Here, the usual splitting in right- and left-moving electrons ($|1,p\rangle \equiv |k_F+p\rangle$, $|2,p\rangle \equiv |-k_F+p\rangle$) been made by means of the Nambu spinors,

$$\begin{aligned} \hat{\psi}_p &\equiv \begin{pmatrix} a_{1,p} \\ a_{2,p} \end{pmatrix}, \\ \hat{\psi}_p^\dagger &\equiv \begin{pmatrix} a_{1,p}^\dagger & a_{2,p}^\dagger \end{pmatrix}, \end{aligned}$$

where $\hat{\sigma}_\pm \equiv (\hat{\sigma}_1 \pm i\hat{\sigma}_2)/2$ ($\hat{\sigma}_{1,2,3}$ — Pauli matrices) and v_F is the Fermi velocity. The $2k_F$ - potential, Δ, acting on electrons consists of two parts,

$$\Delta = \Delta_L + \Delta_i, \tag{7}$$

corresponding to the Peierls distorted lattice (Δ_L) and $2k_F$ - coherent scattering by the $2k_F$ - regularity embodied in the impurity distribution of Equation (4). Their explicit forms read

$$\Delta_L = \frac{1-x}{2} \, A_L \sqrt{\pi v_F \lambda M \omega_Q^2/2} \, \exp[i(\varphi_L + \varphi_g)], \tag{8}$$

$$\Delta_i = \frac{x}{2} \, w_1 \, [V_{e-i}(Q) - V_{e-L}(Q)] \, e^{i\varphi_i} \equiv \frac{x}{2} \, w_1 \, U_B \, \exp[i(\varphi_i + \varphi_B)]. \tag{9}$$

The following notations have been used above: $x \equiv N_i/N$ — fractional impurity concentration, λ — the dimensionless electron - phonon coupling strength, M – mass of host lattice atoms (ions), ω_Q — frequency of the bare $2k_F$ - phonons, φ_g – phase of electron - phonon coupling constant, $V_{e-L}(Q)$ and $V_{e-i}(Q)$ – Q - Fourier

components of electron - lattice and electron - impurity interactions, respectively. The incoherent part, H_{scatt}, comprises both forward and backward scattering of electrons by the random potential associated to the impurity distribution of Equation (4)

$$H_{scatt} \equiv \sum_p \sum_{q \neq 0} \hat{\psi}_{p+q/2}^\dagger \, \hat{U}(q) \, \hat{\psi}_{p-q/2}, \tag{10}$$

$$\hat{U}(q) = \mathcal{U}_F(q)\hat{1} + \mathcal{U}_B(Q+q)\hat{\sigma}_+ + \mathcal{U}_B^*(Q-q)\hat{\sigma}_-, \tag{11}$$

$$\mathcal{U}_F(q) = \frac{1}{L} \sum_{\nu=1}^{N_i} [V_{e-i}(q) - V_{e-L}(q)] \, e^{-iqY_\nu}, \tag{12}$$

$$\mathcal{U}_B(Q+q) = \frac{1}{L} \sum_{\nu=1}^{N_i} [V_{e-i}(Q+q) - V_{e-L}(Q+q)] \, e^{-i(Q+q)Y_\nu}. \tag{13}$$

The last part in the total Hamiltonian, the elastic energy stored by the distorted lattice, is a classical quantity having, in the harmonic approximation, the expression

$$E_{elastic} = \frac{|\Delta_L|^2}{\pi v_F \lambda_L} \, L, \tag{14}$$

where $1/\lambda_L$ is a dimensionless elastic strength renormalized by the presence of impurities. By evaluating the elastic energy in the nearest- neighbour approximation and neglecting impurity-impurity elastic interaction [7] it is of the form

$$\frac{1}{\lambda_L} = \frac{1}{\lambda} \frac{1 - 2x(1 - 1/\alpha)}{(1-x)^2}, \tag{15}$$

where $\alpha \equiv 2(\kappa_{LL}/\kappa_{Li}) \sin^2(Qd/2)$ is a dimensionless quantity essentially proportional to the ratio of lattice-lattice (κ_{LL}) and lattice-impurity (κ_{Li}) elastic strengths. Three effects of impurities on the CDW system are taken into account in the total Hamiltonian written above:

- an extra $2k_F$-potential (Δ_i, Equations (7) and (9)) originating from the coherent scattering of electrons by the $2k_F$- regularity of impurity distribution (Equation (4));
- the usual pair-breaking effect brought about by the incoherent electron – impurity scattering (Equations (10 — 13) via the finite electronic life-time, included in the case of perfectly randomness [6 — 9];

[7] Again, this is justified in the dilute impurity case.

- the renormalization of elastic energy stored up by the Peierls distorted lattice. Although disregarded by the previous studies, this should also be included for perfectly random impurity distribution.

One should remark at this point that the present Hamiltonian differs from that corresponding to the case of displacive motion (Ref. 5) by the forms of the quantities Δ_i (which is no more an independent variational parameter) and $E_{elastic}$ (which does not more contain the interference term dependent on $\varphi_L - \varphi_i$ [5]).

The term H^0, Equation (6), can be treated exactly and its Matsubara (matrix) Green function has the form

$$\hat{G}^0(p,\ i\epsilon) = \left(i\epsilon\ \hat{1} - v_F\ p\ \hat{\sigma}_3 - \Delta\ \hat{\sigma}_+ - \Delta^*\ \hat{\sigma}_-\right)^{-1}.$$

The Born approximation with respect to the term H_{scatt}, Equations (10 – 13), leads to the following self-energy [5, 6, 8, 9]

$$\hat{\Sigma}(p,\ i\epsilon) = \left\langle \sum_q \hat{U}(q)\ \hat{G}(p-q,\ i\epsilon)\ \hat{U}(-q) \right\rangle,$$

where the angular brackets denotes averaging over impurities. Making use of Equation (4), the only non-vanishing averages appearing above are listed below ; assuming furthermore that they are slightly q-dependent one may write

$$\begin{aligned} \langle \mathcal{U}_F(q)\mathcal{U}_F(-q)\rangle &\simeq \frac{x}{dL}\ U_F^2, \\ \langle \mathcal{U}_B(Q+q)\mathcal{U}_B^*(Q+q)\rangle &\simeq \frac{x}{dL}\ U_B^2, \\ \langle \mathcal{U}_F(q)\mathcal{U}_B^*(Q+q)\rangle &\simeq \frac{x}{2dL}\ w_1\ U_F\ U_B\ e^{-i(\varphi_i+\varphi_B)}. \end{aligned} \tag{16}$$

Noteworthy is the non-vanishing value of the last average above, proportional to w_1; it is the direct consequence of the $2k_F$modulated impurity distribution which mixes the forward and backward scattering processes which have the difference of momentum transfers equal to Q (essentially, $2k_F$). The Green function can be expressed as

$$\hat{G}^{-1}(p,\ i\epsilon) = i\tilde{\epsilon}\hat{1} - v_F\ p\hat{\sigma}_3 - \tilde{\Delta}_\epsilon\hat{\sigma}_+ - \tilde{\Delta}_\epsilon^*\hat{\sigma}_-. \tag{17}$$

The set of equations we get in the present case for the quantities $\tilde{\Delta}_\epsilon$ and $\tilde{\epsilon}$, making use of the Dyson equation and the explicit form of the averaged self-energy $\hat{\Sigma}(p, i\epsilon)$

is more complicated than that for the case of either perfect randomness [9] or displacive motion [5], because of the non-vanishing average in the last of Equations (16). Keeping this term, we cannot use the trick employed in Refs.9 and 5; tedious numerical calculations are required. However, one can circumvent this difficulty by inspecting the afore-mentioned set of equations. One can thus see that the method used in Refs. 5 and 9 technically works for either $U_B = 0$ or $U_F = 0$. As concerns the first possibility, one can easily see that it corresponds to the perfectly random case: the contribution of impurity modulation is completely lost, because Δ_i vanishes (cf. Equation (9)). Thus, the modulated impurity distribution merely feels the backscattering processes. We shall therefore restrict ourselves below to the latter case; it has the advantage that the impurity modulation is still retained and a solution in closed analytic form could be given. In this case, the (matrix) Dyson equation leads to the following equations for $\tilde{\Delta}_\epsilon$ and $\tilde{\epsilon}$

$$\begin{aligned} \tilde{\epsilon} &= \epsilon + \frac{\tilde{\epsilon}\ \Gamma_B}{2\sqrt{\tilde{\epsilon}^2 + |\tilde{\Delta}_\epsilon|^2}}, \\ \tilde{\Delta}_\epsilon &= \Delta, \end{aligned} \tag{18}$$

with $\Gamma_B \equiv xU_B^2/v_F d$. One should note than in this case a further simplification arises because of the last equation above. Once the Matsubara Green function is known (Equations (17) and (18)), the thermodynamic potential Ω could easily been obtained as

$$\Omega - \Omega_0 = -2k_BT \sum_p \sum_{i\epsilon} \int_0^{|\Delta|} d\xi \frac{\xi}{\tilde{\epsilon}^2 + v_F^2 p^2 + \xi^2} + \frac{L}{\pi v_F \lambda_L} |\Delta_L|^2, \tag{19}$$

where Ω_0 corresponds to the normal state with perfectly random distribution of impurities. Within the variational approach we adopted here, one has to minimize the above expression with respect to both A_L and $\varphi_L - \varphi_i$.

3 CDW DRIVEN BY MODULATED IMPURITY DISTRIBUTION

We have not yet made any assumption on the fractional modulation amplitude, w_1. We shall assume in this section that w_1 is independent on A_L and the only restriction we impose on it is

$$0 \leq w_1 \leq 1, \tag{20}$$

which ensures a non-negative probability (cf. Equation (4)). The reason why we adopt this model first is two-fold. Firstly, the variational procedure is simpler for this model of w_1. Secondly, although it no more corresponds to a CDW-driven impurity regularity, but rather to a converse situation, where the CDW is driven by the modulated impurity distribution, this situation could also have its own relevance[8]. The minimization with respect to A_L and $\varphi_L - \varphi_i$ then yields the equations

$$\begin{aligned} B \;\; & [|\Delta_L| + |\Delta_i| \cos(\varphi_L - \varphi_i + \delta)] \;=\; \frac{|\Delta_L|}{\lambda_L}, \\ B \;\; & |\Delta_L||\Delta_i| \sin(\varphi_L - \varphi_i + \delta) \;=\; 0, \end{aligned} \tag{21}$$

where B is given by

$$B = \frac{\pi v_F k_B T}{L} \sum_p \sum_\omega \frac{1}{\tilde{\epsilon}^2 + v_F^2 p_2 + |\tilde{\Delta}_\epsilon|^2}, \tag{22}$$

and $\delta \equiv \varphi_g - \varphi_B$. The solution which is energetically the most favoured is $\varphi_i - \varphi_L = \delta$, when $|\Delta| = |\Delta_L| + |\Delta_i|$ and

$$B \;=\; \frac{1}{\lambda_L}\left(1 \;-\; \frac{|\Delta_i|}{|\Delta|}\right). \tag{23}$$

The quantity B can be obtained in the standard method [5, 9, 22] as

$$\begin{aligned} B \;\; &= \;\; B_0 \;+\; \frac{\pi v F k_B T}{L} \sum_p \sum_\omega \left(\frac{1}{\tilde{\epsilon}^2 + v_F^2 p^2 + |\Delta|^2} \;-\; \frac{1}{\epsilon^2 + v_F^2 p^2 + |\Delta|^2} \right), \\ B_0 \;\; &= \;\; \int_0^W \frac{d\xi}{\sqrt{\xi^2 + |\Delta|^2}} \tanh\left(\frac{\sqrt{\xi^2 + |\Delta|^2}}{2\, k_B\, T} \right), \end{aligned} \tag{24}$$

[8] One can remind again in this context the case of KCP [17]. See also Section 4.

where W is the energy bandwidth ($\log(2W/\Delta_0) \;=\; 1/\lambda$) [5].

The dependence on x of Δ at $T = 0$ can be obtained by combining Equations (23) and (24)

$$\begin{aligned} \log \;\; & \frac{|\Delta_0|}{|\Delta|} - \frac{\pi\zeta}{4} + \theta(\zeta - 1)\left\{ \frac{1}{2}\left[\sqrt{1 - \zeta^{-2}} + \zeta \arctan\sqrt{\zeta^2 - 1} \right] - \log\left(\zeta + \sqrt{\zeta^2 - 1} \right) \right\} \\ = \;\; & \frac{1}{\lambda_L}\left(1 - \frac{|\Delta_i|}{|\Delta|} \right) - \frac{1}{\lambda}, \end{aligned} \tag{25}$$

where $\zeta \equiv \Gamma_B/(2|\Delta|)$ and Δ_0 correspond to the clean system.

The non-vanishing expression in the r.h.s. of the above equation reveals the difference between the present result and that derived within the Abrikosov – Gorkov — type approach [6 - 9]. On one hand, there is the contribution of the impurity modulation, reflected in the presence of Δ_i. On the other hand, similar to the case of impurity displacive motion [5], there is also the effect of impurity renormalization of elastic energy, manifested in the difference between λ_L and λ (cf. Equation (15). Figure 1 shows the dependence of A_L on impurity concentration for various values of fractional modulation at $T = 0$. One should remark that, because of the model we have chosen in this section (CDW is now driven by impurity modulation), the quantity Δ does not vanish at increasing x. The true order parameter is now A_L, and it vanishes beyond a certain critical concentration, x_c, which is easily obtained by imposing $A_L = 0$ in Equation (25)

$$\begin{aligned} \log \frac{x_c}{x_{c\,0}} \;\; &= \;\; \frac{1}{\lambda} + \log(2\bar{\zeta}) - \frac{\pi\bar{\zeta}}{4} + \theta(\bar{\zeta} - 1) \\ & \times \;\; \left[\frac{1}{2}\sqrt{1 - \bar{\zeta}^{-2}} + \frac{\bar{\zeta}}{2} \arctan\sqrt{\bar{\zeta}^2 - 1} - \log\left(\bar{\zeta} + \sqrt{\bar{\zeta}^2 - 1} \right) \right], \end{aligned} \tag{26}$$

where $x_{c,0}$ is the critical concentration value in the absence of both impurity modulation and impurity renormalization [6, 8, 9] while, because both Γ_B and Δ_i are proportional to x, $\bar{\zeta} \equiv \Gamma_B/2|\Delta_i|$ is a x-***independent*** quantity.

Notice that in the present case, the equation for the critical concentration possesses a `single value` irrespective of the values of the various input parameters. This

contrasts with the situation encountered in the case of CDW – driven impurity displacive motion; the non-trivial issue there on reentrant CDW behaviour essentially relies upon the fact the critical equation can have several roots [5]. Despite the fact that a reentrant CDW behaviour is no longer possible, a non-monotonic behaviour of A_L with increasing x could occur in the present case for certain (relatively small) values of the electron-phonon coupling strength (λ). This type of behaviour, which is sketched in Figure 2, could reflect itself in elastic (x-ray, neutron, electron) $2k_F$ – scattering data.

The density of states, $N(\epsilon)$, can be obtained in the standard way, from the imaginary part of the Green function [23]. Similar to other situations [5, 9, 22], one gets in the present case that it vanishes in a range of energy $|\epsilon| \leq \Omega_g$ (measured with respect to the Fermi level) where the gap parameter Ω_g has the expression

$$\Omega_g = \begin{cases} |\Delta| \left(1 - \zeta^{2/3}\right)^{3/2} & , \text{ if } \zeta < 1 \, , \\ 0 & , \text{ if } \zeta \geq 1 \, . \end{cases} \tag{27}$$

A *gapless* CDW regime thus exists in the present model. As compared to the Abrikosov-Gorkov — type calculation [9], the range of x compatible to the gapless regime is considerably enlarged, as illustrated in Figure 3. As a way to herald experimentally the gapless regime, the spin susceptibility , χ, can be computed within the ladder approximation for the vertex corrections due to electron-impurity incoherent scattering [5, 9]. Doing so, we get

$$\frac{\chi}{\chi_P} = 1 - \pi k_B T \sum_{u_\epsilon} \frac{1}{|\Delta| \left(u_\epsilon^2 + 1\right)^{3/2} - \Gamma_B/2}, \tag{28}$$

where $\chi_P \equiv 2\mu_B^2/\pi v_F$ is the Pauli susceptibility of the normal 1D metal and $u_\epsilon \equiv \tilde{\epsilon}/|\Delta|$ satisfies the equation

$$u_\epsilon |\Delta| = \epsilon + \frac{\Gamma_B}{2} \frac{u_\epsilon}{\left(u_\epsilon^2 + 1\right)^{1/2}}. \tag{29}$$

In the case $T = 0$ a particularly simple expression is obtained

$$\chi/\chi_P = \sqrt{1 - \zeta^{-2}} \; \theta(\zeta - 1), \tag{30}$$

showing that non-vanishing values of the spin susceptibility in the CDW state exist only in the gapless regime [5, 9]. This is also displayed in Figure 3.

Equations (24), (23), (7 — 9) also provide us with the temperature dependence of the order parameter (A_L in the present case) at various values of impurity concentration (x). [9] The dependence on temperature of A_L can be obtained by solving numerically the afore-mentioned set of equations; it is shown in Figure 4 for two values of the impurity content. Although, as we have just mentioned, there is no CDW – to – normal transition in this model, the order parameter A_L displays a monotonic decrease with increasing T. It eventually vanishes for $T = T_{c,L}$, whose value can be obtained by imposing $A_L = 0$ (alternatively: $\Delta_L = 0$, or $\Delta = \Delta_i$) in Equations (23) and (24), as the solution of the following equation

$$\int_0^W \frac{d\xi}{\sqrt{\xi^2 + |\Delta_i|^2}} \tanh\left(\frac{\sqrt{\xi^2 + |\Delta_i|^2}}{2k_B T_{c,L}}\right) + 2\pi k_B T_{c,L} \sum_{n=0}^{\infty} \left(\frac{1}{\sqrt{\tilde{\epsilon}_n^2 + |\Delta_i|^2}} - \frac{1}{\sqrt{\epsilon_n^2 + |\Delta_i|^2}}\right) = 0, \tag{31}$$

with $\epsilon_n \equiv (2n+1)\pi k_B T_{c,L}$. As compared to both the case of perfect randomness [9] and that of impurity displacive motion [5], the equation for this critical value $T_{c,L}$ is more complicated here because $\Delta = \Delta_i \neq 0$. It can be solved only numerically; the dependence on x of $T_{c,L}$ is illustrated in Figure 5. One should note the large values of $T_{c,L}$ in this case and the possible relation to the physical situations of fictiously (high) critical temperature: besides the case of the compound pioneering the field of quasi-1D materials, KCP, already mentioned (cf. [5] and references therein), this situation reminds on polyacetylene and $(BEDT - TTF)_2 X$, where the dimerization (rather of chemical origin) is not a conventional Peierls distortion (see, e.g. [26]).

[9] A word of caution has to be said at this point, in view of the fact that the present variational approach is basically of mean-field type. Despite the fact that the mean-field temperature is *not* the transition temperature of the real CDW transition, there have been reports showing a satisfactorily good agreement between experiments and mean-field calculations with regards to the temperature dependence up to T — values very close to the real critical temperature [5, 24, 25]. In the case of the model we investigate in this section one may think that the situation is even better, because of the model for w_l the transition to the normal state never occurs.

4 MODULATED IMPURITY DISTRIBUTION DRIVEN BY CDW

The present section is devoted to the discussion of the physical situation — which is more interesting in the light of what was stated in Introduction — where the modulated impurity distribution is driven by the CDW. Then, the quantity w_1 (Equation (4)) is no longer a free input parameter, but depends on the CDW properties. To get this dependence one has to minimize energy of the interaction between impurity distribution and CDW. As the elastic energy does not contain the quantity w_1 (cf. Equations (14,15)), let us evaluate the energy $E_i(Y)$ of interaction between an impurity located at Y and the CDW. Making use of Equations (2) and (9) we get straightforwardly

$$\begin{aligned} E_i(Y) &= \int dx \delta\rho(x) \left[V_{e-i}(x-Y) - V_{e-I}(x-Y)\right] \\ &= \rho_1 U_B \cos\left(QY + \varphi - \varphi_B\right). \end{aligned} \tag{32}$$

Once this interaction energy is known, the thermodynamics requires that the probability of occupying the position Y is ($\beta^{-1} \equiv k_B T$)

$$w(Y) \propto \exp\left[-\beta E_I(Y)\right].$$

If we now assume that there are many impurities in the system but their distribution is dilute enough such that the total energy is the sum of individual terms given by Equation (31) and, according to Equation (3), they only occupy sites in a lattice[10], one obtains the expression

$$w(Y) \propto \exp\left[-\beta\rho_1 U_B \sum_n \cos\left(QY + \varphi - \varphi_B\right) \delta\left(X_n - Y\right)\right]. \tag{33}$$

Now, if the exponent in the above equation is small enough ($\beta\rho_1 U_B \ll 1$), the expansion leads to

$$w(Y) \propto \sum_n \left[1 - \beta\rho_1 U_B \cos\left(QY + \varphi - \varphi_B\right)\right] \delta\left(X_n - Y\right), \tag{34}$$

[10]See also footnote 3.

which is exactly of the form of the Ansatz we made (Equation (4)). If the quantity $\beta\rho_1 U_B$ is not small, by expanding the r.h.s. of Equation (33) we get higher order terms in $\cos(QY + ...)$. However, these terms correspond to higher order harmonics (2Q, 3Q, etc.), which do *not* couple to the purely (co)sinusoidal distortions of the Peierls — CDW state (Equations (1,2)). By still bearing in mind the reason yielding to Equation (20), we are led to Equation (4) with the following expression of w_1

$$w_1 = \begin{cases} \beta\rho_1 U_B & \text{, for } \beta\rho_1 U_B < 1\,, \\ 1 & \text{, for } \beta\rho_1 U_B \geq 1\,. \end{cases} \tag{34 a}$$

As concerns the amplitude of the electronic CDW modulation (ρ_1), it can easily been obtained from the non-diagonal element of the matrix Green function (e.g. [11])

$$\rho_1 = \frac{2|\Delta|}{\pi v_F} B, \tag{35}$$

with B expressed by Equation (22). Obviously, the mismatch in the sign appearing in front of cos in Equations (4) and (34) can be picked up in the phase argument: $\varphi_i = \varphi - \varphi_B + \pi$. In this way, both parameters of the distribution function $w(Y)$ of Equation (4) are entirely specified in terms of the CDW properties.

The minimization of Equation (19), supplemented with Equations (9), (34a) and (35), yields after some calculation the same match in phases as in the preceding case (corresponding to in-phase Δ_L and Δ_I) the self-consistency condition

$$B = \begin{cases} \frac{1}{\lambda_L}\left(\frac{2}{1+\sqrt{1+\frac{4\beta}{\pi\lambda_L}\Gamma_B}}\right)^2 & \text{, for } \frac{2\beta}{\pi v_F}|\Delta| B U_B < 1\,, \\ \frac{1}{\lambda_L}\left(1 - \frac{|\Delta_1|}{|\Delta|}\right) & \text{, for } \frac{2\beta}{\pi v_F}|\Delta| B U_B \geq 1\,. \end{cases} \tag{35 a}$$

Notice that at low temperature the second branch above is "active" and the results we get here are identical to those of Section 3. Actually, the main shortcoming of the treatment in Section 3, insofar the CDW – driven modulation of impurities is intended, is the fact that the CDW does notdisappear by increasing either x or T. Unlike that situation, a transition from the CDW to the normal state occurs in the model we are discussing at the increase of either x or T (explicitly: Δ, Δ_L, $\Delta_I \to 0$ as $x \to x_c$, *or* $T \to T_c$). We therefore claim that the present model realistically

describe the CDW - driven modulated impurity distribution for both low and high (*i.e.* near the CDW transition) temperatures. Because the results we obtain here for low temperatures coincide with those from the preceding Section, we mainly concentrate to the CDW properties near the CDW — normal transition. The temperature dependence of the amplitude A_L, obtained from the above equation, along with that of the gap parameter Ω_g (also given by Equation (27)) is sketched in Figure 6 for a given value of impurity content. As concerns the equation for the critical temperature in the present approach, it is easily obtained by imposing $A_L \to 0$ (alternatively: $\Delta, \Delta_L, \Delta_i \to 0$) in Equation (35) as

$$\int_0^W \frac{d\xi}{\xi} \tanh\left(\frac{\xi}{2k_B T_c}\right) + \sum_{n=0}^{\infty}\left(\frac{1}{n+\frac{1}{2}+\frac{\Gamma_B}{4\pi k_B T_c}} - \frac{1}{n+\frac{1}{2}}\right) = \frac{1}{\lambda_L}\left(\frac{2}{1+\sqrt{1+\frac{4\Gamma_B}{\pi\lambda_L k_B T_c}}}\right)^2 . \tag{36}$$

The dependence on impurity concentration of T_c is displayed in Figure 7. It is worth noting the non-monotonical dependence on x obtained in this model. It contrasts to the overall decreasing CDW critical temperature with increasing impurity content and vanishes at the lower concentration value, $x_{c,0}$ in the perfectly disordered case [6 - 9]. So, similar to the case of displacive motion [5], the value of the CDW critical temperature is ***higher*** when a CDW-driven quasi-regularity is allowed for.

5 DISCUSSIONS AND CONCLUSIONS

As a complementary study of a displacive motion of impurities brought about by CDW [5], we have investigated here the modulated impurity distribution as another kind of quasi-regularity of impurities embedded into the 1D - CDW system. The former study of KCP [17] could be considered as a precursor of the present one. Although a phenomenological inclusion of disorder [27] has supplemented that study, the present investigation goes beyond by a microscopical treatment of disorder and impurity (quasi -) regularity as well as a detailed discussion of the x-dependence of relevant CDW properties. (Of course, there was no need to get this x-dependence

in the case of KCP: the impurity content is fixed in that quasi-1D compound.) One should remark in this context a possible connection between the schematical way of treating the modulated impurity distribution there [17] — which resembles the model of Section 3, of CDW-driven impurity modulation — and the present one: despite the fact that KCP never undergoes a transition to the normal state, the lattice contribution to the quantity denoted here by $|\Delta|$ has a more pronounced decrease with increasing temperature, whereas $|\Delta|$ is practically T - insensitive [28].

As a rule one can state that, whichever the type of $2k_F$ quasi-regularity in the impurity distribution — of either Ref. 5, or Section 3 or Section 4 — , the CDW correlations are enhanced with respect to the case of perfectly random distribution. As discussed previously [5], universal curves for e.g., reduced order parameter, critical temperature and gap parameter as overall ***decreasing*** functions of reduced impurity concentration have been found in the latest case ("law of corresponding states"). Actually, even for perfect randomness, this universality is lost if the impurity renormalization effect is accounted for: it is reflected in the presence of the quantity α in Equation (15). Perhaps the most spectacular manifestation of this loss of universality is the reentrant CDW regime obtained in the case of CDW-driven displacive motion of impurity distribution [5]. Although, as noted in Section 3, a reentrant CDW behaviour is impossible in the case of $2k_F$-modulated impurity distribution, a non-monotonical behaviour of various quantities with increasing x could be displayed in either case of quasi-regularity mentioned above. Experimentally an upturn in the resistive anomaly associated to the upper CDW transition occurring in the linear chain compound $Nb_{1-x}Ta_xSe_3$ at the increase of x beyond ≈ 4.5 % [29]. An analysis of the physical situation in this alloyed quasi-1D compound has recently been made by one of the authors [5] and will be not repeated; we should only remark here that the possible explanation given there by invoking a CDW-driven qnasi-regularity of tantalum atoms could comprise either the displacive motion or the modulated distribution. One should also notice at this point that a non-monotonical change at the variation of impurity content in a physical system

where coexisting ordered phases influence each other is encountered in the heavy fermion superconductor $Th_xU_{1-x}Be_{13}$ (see, e.g. [30], for a recent review) . There a non-monotonical drop of the superconducting critical temperature at the increase of Th content has been observed.

Another similarity with the case of CDW-driven impurity displacive motion we have got here is the possibility of considerably broadening of impurity concentration range for the gapless CDW regime. A gapless CDW state has been observed in heavily ClO_4-doped polyacetylene [26,30], but the range of dopant concentration which is experimentally compatible to the gapless regime is much wider than that obtained for the case of perfect randomness [5]. To assign this broadening to a modulated distribution is particularly tempting in the case of polyacetylene in view of its fictious critical temparature (cf. Section 3).

A non-trivial issue of these investigations of CDW-driven quasi-regularities in the spatial distribution of impurities is the possibility of a thermal hysteretical behaviour at the CDW transition. This behaviour is related to the fact that, when studying the instability of the normal state of the system containing impurities upon cooling, this critical temperature coincides to that of suppressing (by heating) the CDW state with ***perfectly random*** distributed impurities [32]. As already mentioned (see Section 4 and also Ref. 5), the CDW critical temperature is higher in the case of quasi-regular impurity distribution (either displacive motion or modulated distribution). By using in this Section — mainly intended to refer to real (experimental) situations — the corresponding critical values with subscripts related to the way in which the transitions effectively occur, we shall write: [11]

$$T_{heating} > T_{cooling}. \qquad (37)$$

[11] One may think that this inequality is questionable, as for its derivation mean-field — like approximations have been employed. We argue, however, that the physical reason for this inequality goes well beyond these approximations. The engine raising $T_{heating}$ above the value of $T_{cooling}$ is the CDW-driven quasi-regularity; consequently, it acts only when approaching the transition from the CDW side.

Whether the above inequality is effectively observed or not in a system with a presumable modulated impurity distribution strongly depends on at least two things. Firstly, the impurities have to be sufficiently mobile in the host lattice to be able to migrate towards the most favoured positions (cf. the discussion in Introduction). To this aim, one needs a time scale for changing the temperature slower than the time of (atomic) diffusion. Secondly, it is related to the magnitude of critical fluctuations. It seems likely that when they are large, they would reflect themselves in significant ***pretransitional*** effects along with short CDW correlation length. With these in mind, let us proceed by analysing the thermal study on $NbSe_3$ of Ref. 15. Although not very recent and performed on a material not ***intentionally*** [33] doped [12] its salient feature — which makes it particularly suitable for the present analysis — is the fact that this experiment has been conducted with extremely slow variation of temperature: typical rates are $|dT/dt| \approx 1\ K/h$. At such low values of temperature variation, two specific heat anomalies, associated to the partial removal of Fermi surface of this quasi-1D compound due to formations of two CDW gaps [1], have been found [15]. The large pretransitional effects at the upper CDW transition of $NbSe_3$ (up to $\sim 7\ K$) above the critical temperature $T_1 = 145\ K$ [15] combined to the (lower bound) estimation of intrachain CDW coherence length, $\xi_1 \approx 50\ \mathring{A}$ [34] could be inferred to explain why no difference in critical temperature during heating and cooling has been detected in Ref. 15. Fortunately, the lower CDW transition of $NbSe_3$ displays no pretransitional effects [15] and the (lower bound) estimate for the intrachain CDW coherence length is much larger ($\xi_2 \approx 3000\ \mathring{A}$) [35]. One should therefore expect an experimentally detectable difference in the critical temperature at the lower CDW transition. The actual experimental data, $T_{2,heating} = 59\ K$ and $T_{2,cooling} = 58\ K$ [15], agreeing with Equation (37), support the proposed picture. In addition, a finite difference exists at a given temperature T between the values of various quantities (for instance, Δ A_L, Ω_g) computed in the cases where the

[12] The thermal anomalies we are going to discuss in the framework of the proposed model of modulated impurity/defect distribution in these "pure " samples of $NbSe_3$ — which contained, however, a certain amount of intrinsic disorder [33] — are only related to the latest; one would expect larger effects in samples with appropriate (for the present purpose) ***intentional*** doping.

impurity distribution is quasi-regular and perfectly random. In the case where the physical conditions allow a quasi-regular impurity distribution this difference plays no rôle well down from the transition region, as the latter situation is immaterial. However, this difference should yield a first-order character (latent heat) of the CDW transition upon cooling down at the value $T = T_{cooling}$: this is illustrated in Figure 6 by the difference between the solid and dashed lines at $T/T_0 = 1$. It is just the behaviour observed in Ref. 15. The fact that the observed latent heats were much larger than those expected from an incommensurate-commensurate CDW transition is related to the much larger energy scale (of the magnitude order of Δ rather than the pinning frequency) involved in the presently proposed mechanism. [13] So, we interpret the anomalous behaviour (both the hysteresis in the critical temperature T_0 and latent heats) seen in Ref. 15 as due to the fact that the extremely slow change of temperature allows the spatial distribution of defects to follow the CDW and become modulated.

More recently, thermal hysteresis in resistivity and order parameter extracted from x - ray scattering data has been reported in the chain-like compound Ta_2NiSe_7 [36]. It is beyond the present purpose to give a definite picture of the physical behaviour of this material. For this, much more work has to be done from both theoretical and experimental sides. Nevertheless, we think that the present paper, along with the previous ones on quasi-regularity in the distribution of impurities [5, 32] could provide some insight into the unusual features reported in Ta_2NiSe_7 . This is why we shall discuss below in some detail the physical picture emerging from the afore-mentioned study [36]. Let us first summarize the experimental findings in this material, as stated by the investigators of Ref. 36. An electronic anomaly and an incommensurate modulation have been observed in Ta_2NiSe_3 . It has been concluded that the structural distortion is of electronic origin (i.e. a CDW); however,

[13] One of the motivations for this investigation was to understand the anomalous thermal behaviour reported in [15] for unintentionally doped $NbSe_3$. The reason we displayed in all Figures the various curves for very small values of impurity concentration is to evidence the fact that, even then, the various effects discussed are physically significant.

some unusual features found there do not rule out a chemical origin of the distortion. It has been also claimed that the much more ordered structure of Ta_2NiSe_7 with respect to its structurally similar compound $FeNb_3Se_{10}$ drastically reduces the magnitude of the (impurity-like) random potential present in the latter. Consequently, one may expect a metallic behaviour of Ta_2NiSe_7 over a broad temperature range starting from room temperature and extending down to liquid hellium. However, from these measurements it was inferred that the ordering (of Ni and Ta on the octahedral chains) is incomplete. As such, a weak localization remains at low temperatures. As in $FeNb_3Se_{10}$, the disorder present in Ta_2NiSe_7 affects the formation of true long-range order below the CDW onset temperature and the amplitude of CDW, not just the phase as in other compounds with chain or layered structure. Three main observations have led the authors of Ref. 36 to conclude that a CDW is formed in Ta_2NiSe_7: a resistive anomaly, a magnetic susceptibility anomaly and x-ray scattering satellite intensities (corresponding to an incommensurate CDW). Roughly, all these anomalies develop in the same temperature region. The resistive anomaly, whose shape is qualitatively similar to that of $NbSe_3$, though of smaller magnitude, has its upturn at the temperature $T_o = 52.5\ K$, suggesting the CDW onset at that temperature. The anomaly in magnetic susceptibility data is much smaller than that in resistivity. The smallness of these anomalies witnesses the fact that the CDW formation removes but a small part of the Fermi surface; only a reduced fraction of carriers is affected. The T - dependent integrated intensity of the x-ray (incommensurate) CDW satellite [14] displays a number of unusual features [15 16], but what matters at the present stage of discussion is that, essentially, it accompanies the afore-mentioned anomalies in the same temperature range. More interesting for the present purpose is the clear observation of thermal hysteresis. The resistivity

[14] This is usually taken as a measure of the squared CDW order parameter.

[15] For instance: it extrapolates to zero at a value — normally defining experimentally the CDW critical temperature — which difers from T_o specified above; the peak intensity is higher at $55.7K(> T_o)$ than at $51.8K(< T_o)$.

[16] Actually, the analysis of the x-ray data in Ref. 36 relies upon the assumption of a single distorted subsystem. A reexamination of this analysis should be neccessary whether, as we are going to suggest, an overimposed quasi-regularity exists. In addition, even in a conventional situation, there could be satellite intensities above the transition due to the precursor phonon softening.

is larger upon warming than upon cooling, implying thereby a *larger* CDW gap during *warming*: exactly the behaviour we expect in the case of a quasi-regular impurity distribution (of either the kind discussed in this paper or that of displacive motion kind [5]). Most encouraging for such an interpretation is the fact that a hysteresis in the very x-ray scattering intensities — thus *directly* associated to a *modulated* structure — accompanies the thermal hysteresis in resistivity. Furthermore, the coincidence of temperature ranges rules out the possibility to ascribe the latter to the difference in local readjustment of CDW phase during warming and cooling. Along the same line, one should claim that the CDW phason contribution to the conductivity (and, thence, resistivity hysteresis) plays no rôle, as the attempts to detect non-linear conduction below the CDW transition region failed [36].

More generally, one can assign the present work as investigating the possibility of a CDW-driven ordering in a system which is manifestly disoredred. We mention in this context a recent study [37] — from the experimental side this time — which pretty fits this more general framework. There, by employing high-resolution electron microscopy in investigating the Ag – Mg alloys near Ag_3Mg, the formation of long-period superlattice structures from the disordered phase has been observed. A CDW-driven ordering process has been suggested, related to the nesting property of the Fermi surface.

In these phenomena involving quasi-regularities induced by an ordered (CDW) phase, the explicit inclusion of impurity kinetics (diffusion processes) - in the way discussed in [38] — would be a desirable next step.

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FIGURE CAPTIONS

Figure 1: Amplitude of the lattice distortion, A_L, normalized to that of the clean system, A_0, plotted versus impurity concentration, x, at $T = 0$ for several values of fractional modulation: dash — $w_1 = 0$ (perfect randomness), solid — $w_1 = 0.2$, dash-dot — $w_1 = 0.5$ and dash-double dot — $w_1 = 1$. The value $x_{c,0}$ represents the critical concentration value in the absence of modulation and impurity renormalization effect. The values of model input parameters are: $\alpha = 0.5$, $\overline{\zeta} = \sqrt{1000}$, $\lambda = 0.25$ and $x_{c,0} = 10^{-4}$. Notice the increase in A_L with increasing modulation parameter (w_1). (Case of modulated impurity distribution independent of CDW.)

Figure 2: Dependence on reduced impurity concentration ($x/x_{c,0}$) of normalized amplitude of lattice distortion (A_L/A_0) at $T = 0$ for several values of electron-phonon coupling strength: dash — $\lambda = 0.30$, dash-dot — $\lambda = 0.25$, solid — $\lambda = 0.22$, dash-double dot — $\lambda = 0.20$ and dot-double dash — $\lambda = 0.19$. The values of remaining input parameters are: $\alpha = 0.5$, $\overline{\zeta} = \sqrt{1000}$, $x_{c,0} = 10^{-4}$ and $w_1 = 1$. Noteworthy is the *non-monotonical* behaviour in a certain range of λ-values as well as the non-vanishing A_L values well beyond the critical impurity content in the case of perfect randomness ($x \gg x_{c,0}$). (Case of modulated impurity distribution independent of CDW.)

Figure 3: Normalized order parameter (A_L/A_0), gap parameter ($\Omega_g/|\Delta_0|$) and spin susceptibility (χ/χ_P) plotted versus reduced concentration ($x/x_{c,0}$) for $\alpha = 0.5$, $\overline{\zeta} = \sqrt{1000}$, $\lambda = 0.25$ and $w_1 = 1$ at $T = 0$. (Case of modulated impurity distribution independent of CDW.)

Figure 4: Temperature dependence of the order parameter A_L normalized to the value A_0 corresponding to the clean system at zero temperature. The input parameters values are: $\alpha = 0.5$, $\overline{\zeta} = \sqrt{1000}$, $x_{c,0} = 10^{-4}$, $\lambda = 0.30$, $w_1 = 1$ and: $x/x_{c,0} = 0.01$ — dashed line and $x/x_{c,0} = 1.0$ — solid line (T_0 — mean-field critical temperature of the clean system). (Case of modulated impurity distribution independent of CDW.)

Figure 5: Dependence of the temperature T at which the distorted lattice amplitude vanishes ($A_L = 0$) (denoted by $T_{c,L}$ in the main text) on impurity concentration x. T_0 and $x_{c,0}$ have the same meaning as in the preceding Figures. The large values of T are the consequence of the fact that the transition to the normal state never occurs in the model where w_1 is independent of CDW properties. The employed parameter values are: $\alpha = 0.5$, $\overline{\zeta} = \sqrt{1000}$, $x_{c,0} = 10^{-4}$, $w_1 = 1$, and: $\lambda = 0.25$ — solid line and $\lambda = 0.30$ — dashed line.

Figure 6: Dependence on temperature of the normalized lattice distortion amplitude A_L/A_0 (dashed line) and normalized gap parameter $\Omega_g/|\Delta_0|$ (dotted line) for the case of CDW-driven modulated impurity distribution. In the T – range where a single (dotted) line appears, the curves are indistinguishable. For comparison, the solid line, showing the T – dependence of A_L/A_0 in the case of perfect randomness is also given. (A_0 and Δ_0 are specified in the preceding Figures.) The parameters α, $\overline{\zeta}$, $x_{c,0}$, and λ have the same value as in Figure 4, while $x/x_{c,0} = 0.01$. The inset details the difference between the afore-mentioned curves for temperatures beyond T_0.

Figure 7: Critical temperature T of the CDW – to – normal transition occurring in the case of CDW-driven modulated impurity distribution (denoted by T_c in the main text) plotted versus impurity concentration. The meaning and values of input parameters are the same as in Figure 5. Notice the *non-monotonical* x-dependence of the critical temperature.

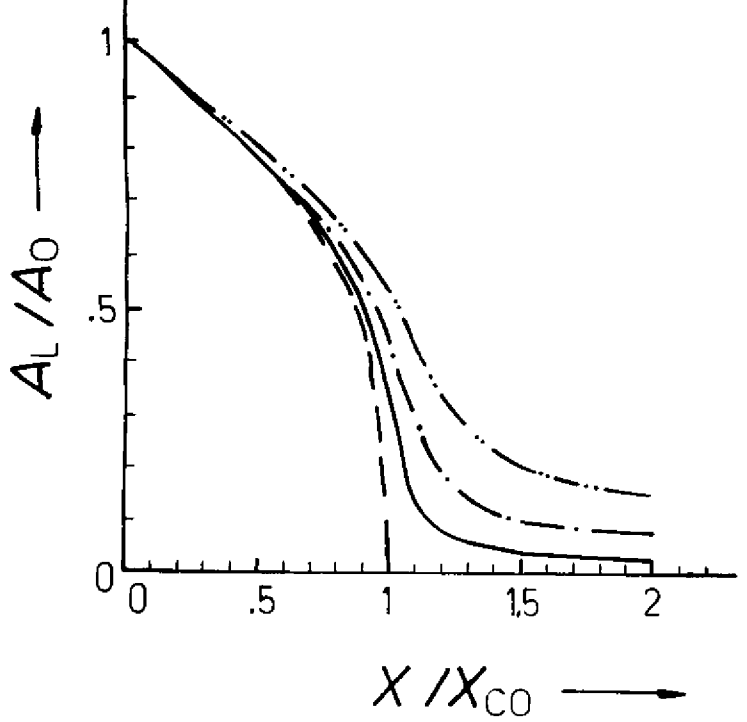

Fig.1

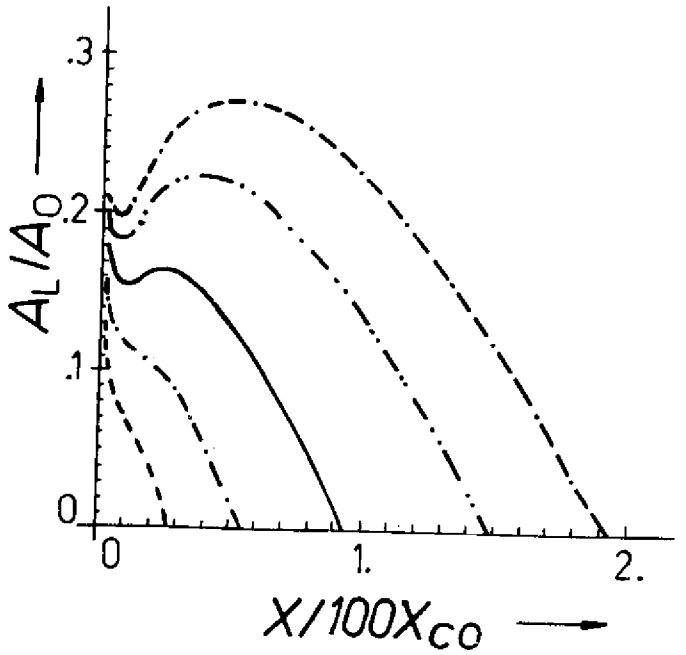

Fig.2

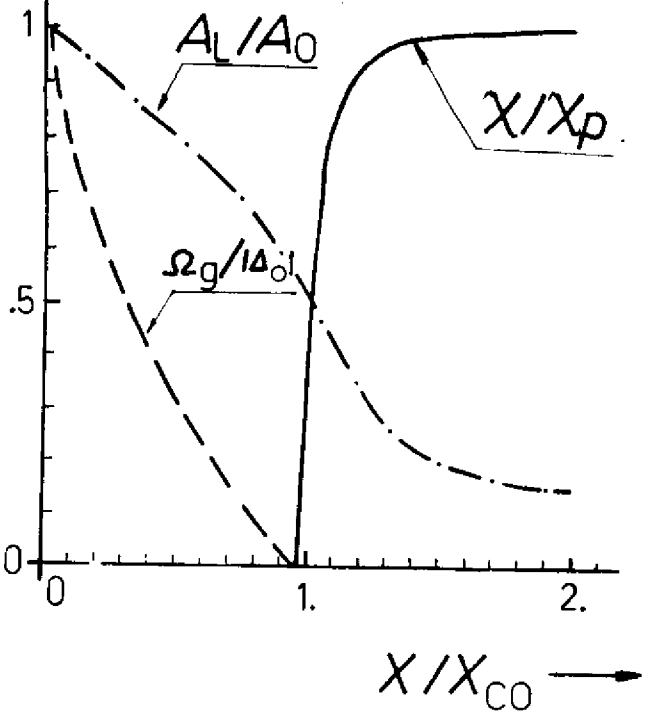

Fig.3

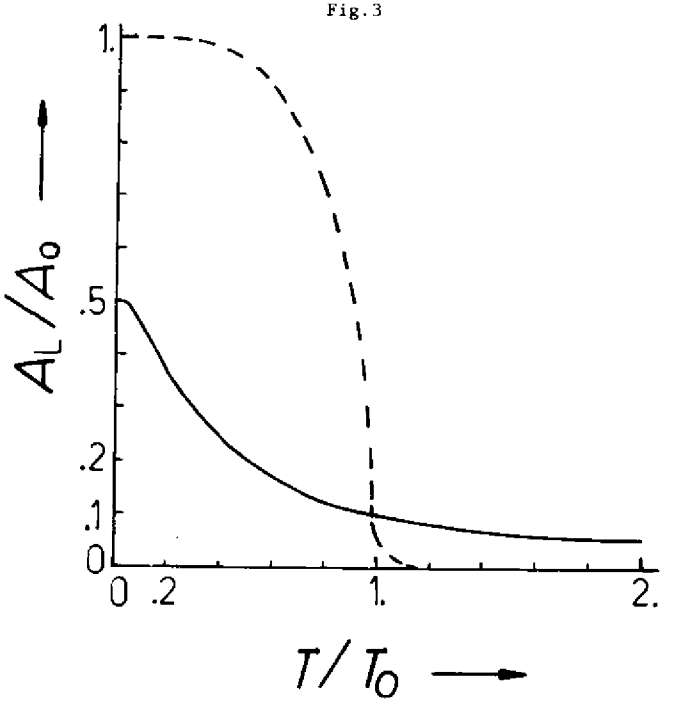

Fig.4

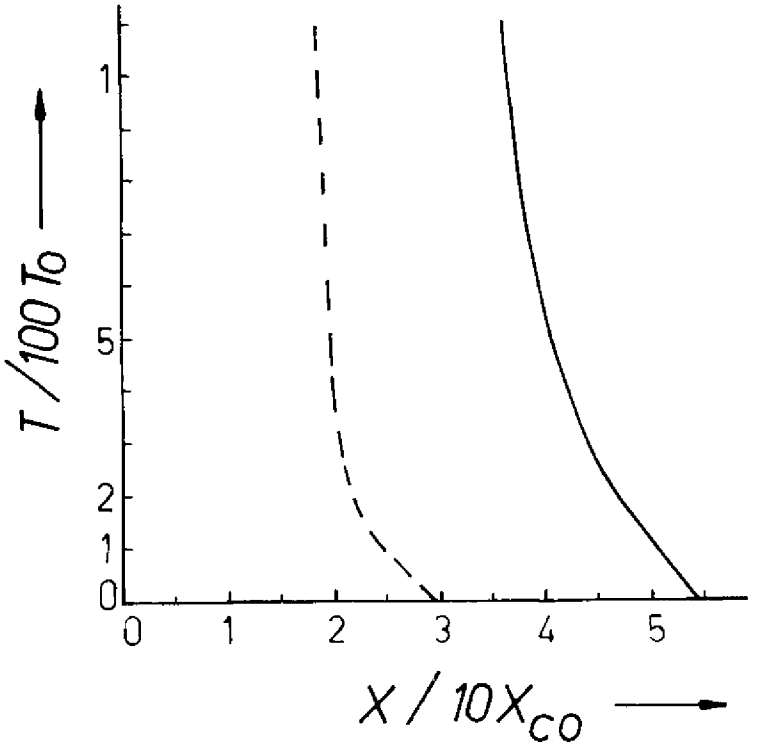

Fig.5

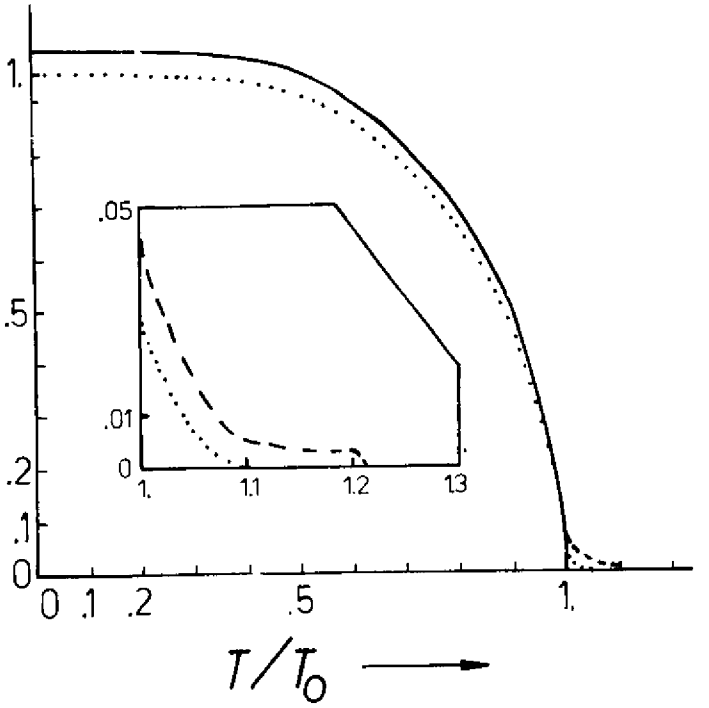

Fig.6

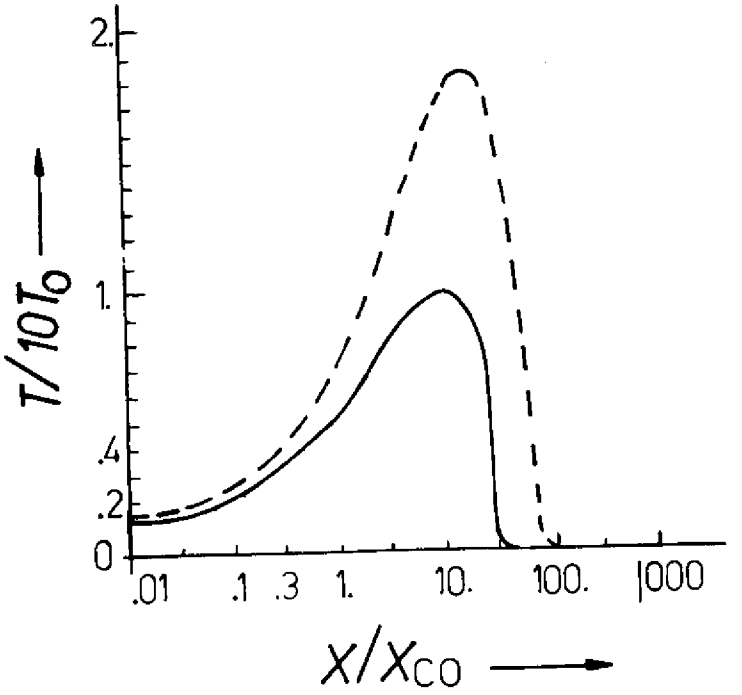

Fig.7