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CDW screening of the charged impurity

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Résumé. — Nous décrivons le mécanisme d'écrantage d'une impureté chargée par l'onde de densité de charge (ODC). Les porteurs de charge se détachent de l'impureté, entrent dans le réseau de l'ODC et se situent au voisinage de l'impureté. Ceci résulte en la création d'une boucle de dislocations dans le réseau de l'ODC. Les chaînes avec les charges supplémentaires portent les solitons 2π , associés aux états électroniques localisés. Cette description d'écrantage est obtenue à partir de l'approximation continue pour les déformations du réseau de l'ODC.

Abstract. — A mechanism of screening of the charged impurity by the CDW is described. The carriers released by the impurity are absorbed by the CDW lattice and situated around the impurity. This results in the creation of the dislocation loop in this lattice. The chains with additional charges carry the 2π solitons, which provide for the localized electronic states. The described screening picture is derived using the continuous approximation in the treatment of the deformations of the CDW lattice.

1. Introduction.

Interaction between the impurity and the charge density wave (CDW) in the quasi one-dimensional systems was much studied in the past [1-5]. The reason is that the impurities are inhibiting the Fröhlich conductivity, contributing to the threshold field for the CDW conduction and possibly to the periodic fluctuations (periodic noise) of the CDW current. In most approaches [1-5] to these problems the impurities (treated either as weak or as strong perturbations of the CDW) are assumed to be neutral. The usual argument is that they are screened by the small pockets of the free electrons, which subsist in the CDW phase. However it became clear recently that in some systems [7, 8] like ortho TaS₃ or blue bronzes the free electrons are very scarce at low temperatures. The charged impurities can then be screened only by the CDW itself [9]. It will be argued here [10] that this screening may be described on combining the well known concepts of local charge neutrality [11], quasi one-dimensional CDW lattice [12] and (its [13]) dislocations [14].

2. Deformations and charge densities.

Quasi one-dimensional systems often exhibit the tendency towards a spontaneous formation of the $2k_F$ charge oscillations (CDW's). The latter are usually coupled to the lattice displacements. The coupled CDW/lattice system is then described by the displacement

$$u_n(x) = |\psi_n(x)| \cos [2k_F x + \mathbf{Q}_\perp \cdot \mathbf{R}_n + \phi_n(x)]. \quad (1)$$

Here $\mathbf{R}_n = d_\perp (n_y \mathbf{j} + n_z \mathbf{k})$ and $(2k_F \mathbf{Q}_\perp)$ is the wave-vector of the spontaneous CDW/lattice condensate described by the complex order parameter $\psi = |\psi| \exp(i\phi)$. $n_{y,z}$ are the indices of the chain which stretches along the x direction.

The impurity pins down the phase $\phi_n(x)$ of $\psi_n(x)$ and deforms $\psi_n(x)$ itself [1-5]. The deformations of ψ are related in particular to the redistribution of the CDW charge $\rho_n^{\text{CDW}}(x)$. This relation has to be established with some care : the charge density of the lattice and the impurity is

$$\rho_n(x) = \rho_0 + Z\delta_{n_0} \delta(x), \quad (2)$$

where Z is the relative valence of the impurity and ρ_0 the average ionic density. It is therefore convenient to separate $\rho_n^{\text{CDW}}(x)$ in

$$\rho_n^{\text{CDW}}(x) = \rho_0 + \rho_n^s(x) + \rho^f \cos [2k_F x + \mathbf{Q}_\perp \cdot \mathbf{R}_n + \phi_n(x)], \quad (3)$$

where $\rho_n^s(x)$ collects the slow variations of ρ^{CDW} and ρ^f is the amplitude of its fast $2k_F$ component. The value of $2k_F$ is given by ρ_0 . The contributions (3) to ρ^{CDW} have been evaluated by various methods, including the diagrammatic expansions [15, 16] and the phase shift approach [16, 17]. The result is that

$$\rho_n^s(x) \simeq \frac{-i}{4\pi|\psi_0|^2} \left(\psi_n^* \frac{\partial \psi_n}{\partial x} - \psi_n \frac{\partial \psi_n^*}{\partial x} \right) + C \quad (4)$$

per spin, where $|\psi_0|$ is the equilibrium value of $|\psi|$ at $T=0$ while ρ^f is linear in $|\psi|$. The charge conservation between equations (2) and (3) requires that

$$Z = 2 \sum_n \int \rho_n^s(x) dx, \quad (5)$$

the factor of two coming from spin.

Equation (5) is the analog of the Friedel sum rule [11] and the last term in equation (3) is reminiscent of the Friedel oscillations, which however are decaying at large distances in electronically isotropic systems. The analogy is particularly transparent if equation (4) is associated with the phase shift approach [16, 17], as will be argued later.

Equation (5) determines the constant C in equation (4). If at large distances $\rho_n^s(x)$ tends to a finite value a part of the charge Z released by the impurity into the CDW remains extended over the whole crystal. Otherwise it is all localized around the impurity.

3. CDW energy.

The overall Coulomb energy of the positive and negative charges ρ_0 in equations (2) and (3) vanishes. $\rho_n^{\text{CDW}}(x)$ couples thus to the impurity through

$$H_{\text{imp}} = -Ze^2 \sum_n \int v_n(x) (\rho_n^{\text{CDW}}(x) - \rho_0) dx, \quad (6)$$

i.e. the slow and fast Fourier components of $\rho_n^{\text{CDW}}(x)$ couple respectively to the slow and fast components v_f^s of the impurity potential $v_n(x)$. At large distances

$$v_n^s(x) = \frac{1}{[x^2 + \epsilon_\Delta R_n^2]^{1/2}}, \tag{7}$$

with $R_n^2 = y^2 + z^2$. In equation (7)

$$\epsilon_\Delta = 1 + k_{\text{TF}}^2 \xi_f^2, \tag{8}$$

is the dielectric constant along the chain of the semiconductor [9, 18] with the gap proportional to ξ_f^{-2} . ξ_f is the low temperature CDW correlation length and k_{TF} is the Thomas-Fermi wavevector of the corresponding [9, 19] metal. Weak couplings are assumed all throughout [9], which amounts [19] in particular to $k_{\text{TF}}^2 d_\perp^2 < 1$.

Analogously to equation (6) the Coulomb energy of the CDW charges is [9]

$$H_c = \frac{e^2}{2} \sum_{nm'} \int dx dx' v_{nm'}^s(x-x') \rho_n^s(x) \rho_{n'}^s(x). \tag{9}$$

Simultaneously with that the energy of the coupled electron-lattice system at $T = 0$ is approximately [9]

$$H_{\text{ep}} = A' \sum_n \int \left[-|\psi_n^2| + \frac{B}{A'} |\psi_n^4| + \xi_f^2 \left| \frac{\partial \psi}{\partial x} \right|^2 + \xi_\perp^2 d_\perp^{-2} |\psi_n - \psi_{n+1}|^2 \right] dx. \tag{10}$$

The coefficients A' and B are related to the presumably small electron-phonon and Coulomb couplings [9], while ξ_\perp describes the weak interchain interaction [9, 12] of the $2k_F$ deformations or CDW's.

Using equation (4) all energies in question can be expressed in terms of ψ . Minimizing with respect to $\phi_n(x)$ while keeping $|\psi|^2 = |\psi_0|^2 = A'/2B$ leads to

$$\xi_f^2 \frac{\partial^2 \phi}{\partial x^2} + \xi_\perp^2 \left(\frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) = \frac{1}{4} k_{\text{TF}}^2 \xi_f^2 \frac{\partial}{\partial x} \int d\mathbf{r}' \rho^s(\mathbf{r}') v^s(\mathbf{r} - \mathbf{r}') - \frac{Z}{4} k_{\text{TF}}^2 \xi_f^2 d_\perp^2 \left[\frac{\partial v^s(\mathbf{r})}{\partial x} + v_f \rho^f \sin \mathbf{Q} \cdot \mathbf{r} \right]. \tag{11}$$

The continuation in the transverse direction has been performed here after expanding equation (10) according to

$$2 \cos(\phi_n - \phi_{n-1}) - 2 \simeq (\phi_n - \phi_{n+1})^2 \simeq d_\perp^2 (\nabla_\perp \phi)^2. \tag{12}$$

The phase only equation (11) is somewhat simpler than its counterpart with varying amplitude, especially because equation (4) reduces now to

$$\rho^s(\mathbf{r}) = \frac{1}{2\pi} \frac{\partial \phi(\mathbf{r})}{\partial x} + C. \tag{4'}$$

Equation (11) is sufficient for present purposes. In this respect it is also convenient to express it in terms of the Fourier components ϕ_q of the phase

$$\phi_q (\xi_f^2 q_\parallel^2 + \xi_\perp^2 q_\perp^2 + k_{\text{TF}}^2 \xi_f^2 q_\parallel^2 v_q^s) = \frac{Z}{4i} k_{\text{TF}}^2 \xi_f^2 d_\perp^2 (q_\parallel v_q^s - i \rho^f v_f^1) \tag{13}$$

where $v_q^s = (\varepsilon_\Delta q_\parallel^2 + q_\perp^2)^{-1}$ and v_f^l is the imaginary part of the fast Fourier component v^f of the impurity potential. Equation (13) reduces to the usual form [2] if only the fast components are retained. Here we shall consider the opposite limit $q_\parallel v_q^s \gg v_f^l$.

4. Free chains.

It is instructive to discuss first the case of elastically uncoupled chains [9], $\xi_\perp = 0$ in equation (13). Noting that according to equation (4') $i q_\parallel \phi_q$ is the displaced CDW charge it is possible [9] to extract the longitudinal dielectric constant ε_L of the composite CDW/semiconductor system from equations (13) and (8),

$$\varepsilon_L = \frac{1}{q_\parallel^2 + q_\perp^2} [\xi_\parallel^2 k_{TF}^2 q_\parallel^2 + q_\perp^2 + k_{TF}^2]. \quad (14)$$

At small q the impurity is screened in the Thomas-Fermi fashion. The screening distances $\lambda_{\parallel, \perp}$ along and transverse to the chains are respectively [9]

$$\begin{aligned} \lambda_\parallel &\approx \xi_\parallel \\ \lambda_\perp &\approx k_{TF}^{-1}. \end{aligned} \quad (15)$$

The transverse screening distance λ_\perp is the same as in the metallic phase, while λ_\parallel is considerably longer. When $\lambda_\perp \approx d_\perp$ the screening cloud is mostly (but never entirely) localized on the impurity chain itself. The exponential decay of $\phi(\mathbf{r})$ introduces however quite large transverse gradients $\nabla_\perp \phi$ and it is therefore appropriate to discuss next the role of the transverse coupling ξ_\perp .

5. Elastically coupled chains.

The term $\xi_\perp^2 q_\perp^2$ in equation (13) becomes important when larger than $\xi_\parallel^2 q_\parallel^2$ and $\xi_\perp^2 \varepsilon_\Delta q_\parallel^2$. It is therefore interesting to find $\phi(x)$ at large distances x along the $y = z = 0$ impurity chain. The Fourier transform gives

$$\phi_p(x) \approx Z - \frac{k_{TF} \xi_\parallel d_\perp^2}{8 \xi_\perp} \frac{1}{x} \left[1 - \exp\left(-\frac{|x| k_{TF} \xi_\perp}{\xi_\parallel}\right) \right] \quad (16)$$

using the weak coupling assumption $k_{TF}^2 d_\perp^2 < 1$ and assuming in addition that $\xi_\parallel^2 > \xi_\perp^2 \varepsilon_\Delta$, i.e. $k_{TF}^2 \xi_\perp^2 < 1$ according to equation (8). $\phi(x)$ vanishes at large $|x|$ which means through equation (4') that there is no charge localization around the impurity on the impurity chain. The corresponding charge distribution is sketched in figure 1. From equation (16) it is clear that the charge deconfinement and the ensuing lack of screening are due to the nonvanishing transverse elastic coupling ξ_\perp , which does not allow for transverse phase gradients at large distances. Such deconfinement effect of ξ_\perp was already encountered during the study of soliton stability in systems of elastically coupled chains [20].

It should be realized however that the solution (16) of equation (11) is not unique. This is best understood if on following Friedel, the two v^s terms in equation (11) are combined in an effective field. The solution of the resulting equation consists of a solution ϕ_L of the homogeneous (Laplace) equation added to a particular solution of the effective field problem. The free coefficients should then be determined selfconsistently with the effective field. Several iterations may be required. In the first step of this procedure we choose to combine

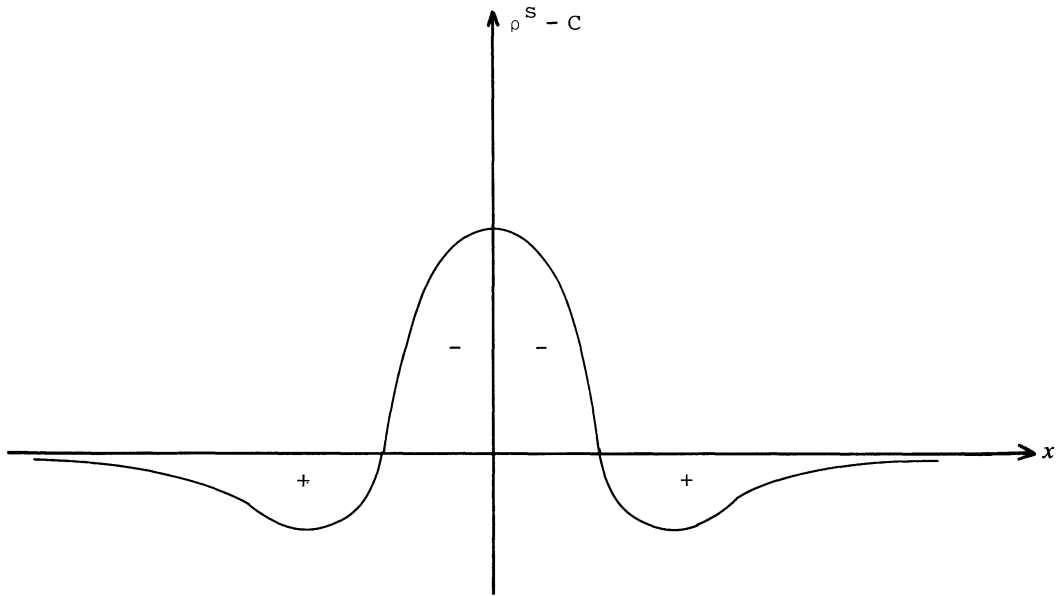


Fig. 1. — Charge distribution corresponding to equation (16).

ϕ_p of equation (16) with the approximate solution of the Laplace equation, appropriate at large distances

$$\phi_L = m \left[\text{Arc tan} \frac{\xi_{\perp} x}{\xi_{\parallel} (\rho + \rho_0)} - \text{Arc tan} \frac{\xi_{\perp} x}{\xi_{\parallel} (\rho - \rho_0)} \right] \tag{17}$$

where $\rho^2 = y^2 + z^2$, ρ_0 is a constant and m is an integer. This latter follows from the requirement that $\psi = |\psi| \exp(i\phi_L)$ is a single valued function of \mathbf{r} even though ϕ_L is not. For $\rho < \rho_0$, ϕ_L behaves as

$$\phi_L \approx m \left(\pi - \frac{\rho_0 \xi_{\parallel}}{|x| \xi_{\perp}} \right) \text{sign } x \tag{18}$$

whereas for $\rho > \rho_0$ it tends towards a constant, as shown in figure 2. This result obtained here in the continuous limit has a particularly simple interpretation in terms of (transversely) discrete chains. When projected on such chains ϕ_L corresponds to a 2π solitons on each chain within ρ_0 around the one which contains the impurity. The chains beyond ρ_0 are essentially unperturbed. This is summarized in figure 3.

The transverse elastic energy of the described configuration is small. This follows from equations (10) and (12). In the discrete version, figure 3, the transverse energy between the soliton chain and the adjacent chain unperturbed at large x , is proportional to $\cos^2 2\pi - 1 \approx 0$. In the continuous version used to derive equation (17), ϕ_L must be taken as multivalued function, figure 2, on circling around the $x = 0, \rho = \rho_0$ line. Again $(\nabla_{\perp} \phi)^2$ is small. It should be also noted in this respect that at large x $\phi_p + \phi_L$ has a lower transverse elastic energy than ϕ_L itself, due to the partial cancellation of the $1/x$ term between equations (16) and (18). $\phi_p + \phi_L$ reaches faster the values $\pm \pi$. Moreover it will be argued below that by perfect screening ϕ_L may also make the Coulomb energy small.

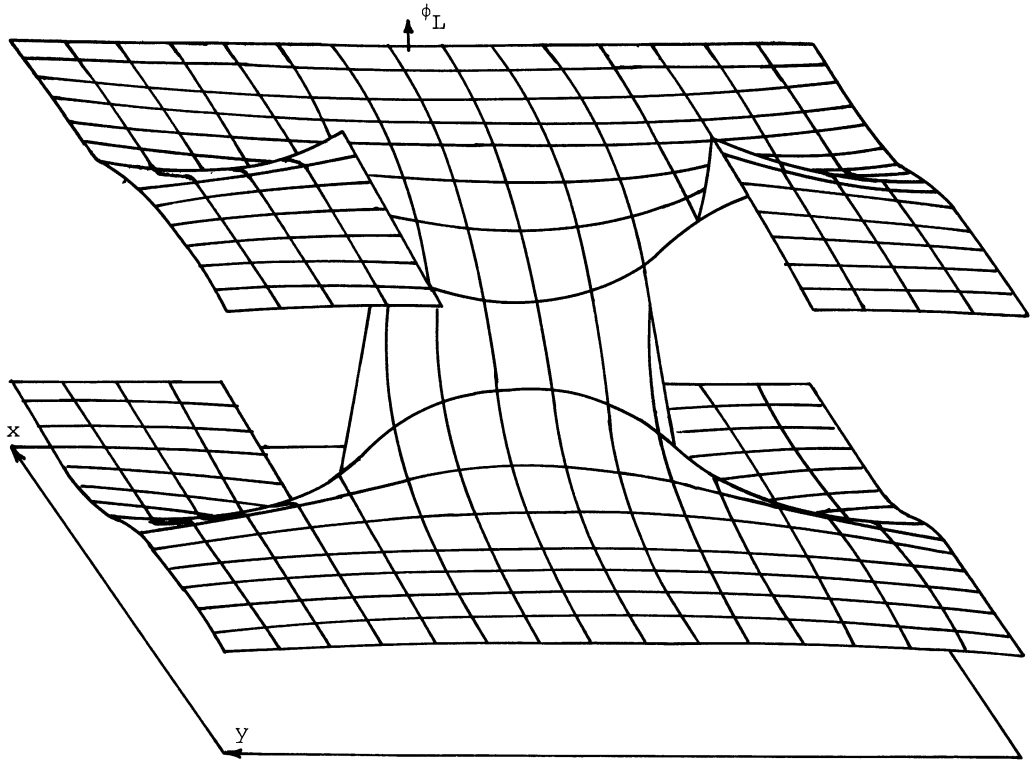


Fig. 2. — Multivalued function $\phi_L(\mathbf{r})$ of equation (17) continuous on circling around singularities.

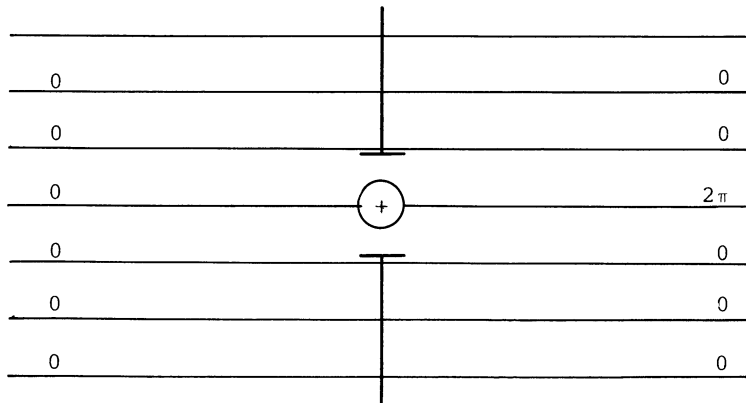


Fig. 3. — 2π soliton on the impurity chain free of interchain elastic coupling.

Before turning to the question of screening let us add two remarks. The first concerns the amplitude variations. The configuration of the phase described above corresponds to a dislocation loop in the CDW lattice at $\rho = \rho_0, x = 0$ where equation (17) is singular. As is well known the amplitude $|\psi|$ of the order parameter must vanish on such singularity line [13]. This is why equations (4), (6) and (9) are written to allow for the variations of the

amplitude. They show in particular that the asymptotic behaviors beyond the distance $\xi_{\parallel}/\xi_{\perp} k_{TF}$ characterizing the present problem in equation (16), are not affected by the amplitude variations, which occur over the shorter distances ξ_{\parallel} , ξ_{\perp} . Moreover, in the discrete case of figure 3 the zero of the amplitude falls naturally between the chains.

Further on, it should be realized that the physical picture of 2π solitons attached to the impurity, derived from the approximate solution (17) of the Laplace equation, is in fact independent of the approximation in question. This is best seen if the same problem is considered in two dimensions, where the solution (17) with y instead of ρ is an exact solution of the Laplace equation. In the continuous limit it describes the two Kostelitz-Thouless vortices at distance $y = \pm \rho_0$ from the impurity. Figure 3 corresponds in fact to this case. The corresponding discrete picture again exhibits the 2π solitons between the two vortices and the essentially unperturbed lattice beyond.

6. Screening.

The coefficients m , ρ_0 in equation (17) should be determined in principle by the minimization of the total energy after inserting $\phi_p + \phi_L$ into equations (6), (9) and (11). Instead a somewhat simpler but more intuitive approach is adopted here. After having argued that the transverse elastic energy of $\phi_p + \phi_L$ is small it will be shown here that this configuration may provide for a perfect screening i.e. minimize the Coulomb energies (6) and (9) too. According to equation (4) or (4') the local neutrality requirement of equation (5) is fulfilled with ϕ_L of equation (18) provided that

$$Z = 2mN, \quad (19)$$

where $N \approx 2\pi\rho_0^2/d^2$ is the number of chains which carry a 2π soliton with the screening charge $2m$ in the vicinity of the impurity. Note that equation (4) allows also for amplitude variations. It shows that they do not affect the result (19) in an essential way.

Further discussion of equation (19) depends somewhat on the value of Z . A few representative cases will thus be considered below :

$Z = 2$. The simplest situation occurs for $Z = \pm 2$ when $N = 1$ and $m = \pm 1$ in equation (19). Figure 3 illustrates just this situation. The 2π soliton on the impurity chain carries $2m = 2$ local charges, one of each spin.

$Z = 1$. Taken at its face value equation (19) means that only even Z 's can be screened by the CDW. The π soliton which would screen $Z = 1$ according to equation (4), is forbidden by the transverse coupling ξ_{\perp} . In order to understand what happens it is then useful to consider the electron level structure in presence of the 2π soliton. The latter is shown in figure 4. The 2π soliton extracts two states (one per spin) from the conducting band of the chain and brings them close to the top of the filled valence band [21]. When the unique impurity electron is put in those states it adds to the soliton a local charge equal to unity [17]. A factor of 2 is therefore removed from equations (5) and (19) and the full screening of the impurity charge $Z = 1$ is achieved. This clarifies the origin of the difficulty : equation (4) corresponds to a filled local state [17] and equation (5) as it stands, assumes that both local states are occupied.

Obviously, the present $Z = 1$, argument can be extended to any odd Z .

Large Z . In the somewhat academic limit of large Z there is some ambiguity in choosing m and N in equation (19) and even it is not clear that m should be equal on all chains. The best choice from the point of view of the transverse elastic coupling ξ_{\perp} seems to be the elimination of the $1/x$ term between equations (16) and (18). This leads to $\rho_0 \approx \max(\xi_{\perp}, d_{\perp})$ i.e. $d_{\perp} \sqrt{N} = \max(\xi_{\perp}, d_{\perp})$. Such choice of ρ_0 is also favorable to the Coulomb energy, when it coincides with the value of the transverse screening length λ_{\perp} of equation (15). Otherwise some intermediate choice of m and N might be preferable.

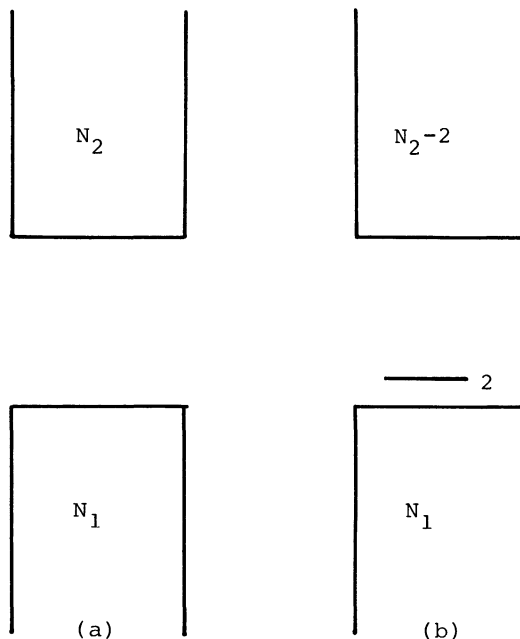


Fig. 4. — Numbers of states in (a) undeformed valence and conduction band (b) in presence of a 2π soliton.

7. Conclusion.

It has been argued here that the CDW can screen the impurity by attaching to it and appropriate number of the $\pm 2\pi$ (anti) solitons on the neighboring chains. This leads to the full screening of the impurity, i.e. the crystal is locally neutral at large distances from the impurity. The structure which results in the $2k_F$ CDW lattice is the dislocation loop perpendicular to the chain direction, with the impurity chain in the center.

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