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PINNING OF AMPLITUDE SOLITONS IN PEIERLS SYSTEMS WITH IMPURITIES

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1. INTRODUCTION

As is well known in Peierls systems with half-filled bands the ground state is two-fold degenerative. This degeneration appears as a result of the lattice dimerization which is caused by the structural phase transition due to the electron-phonon interaction (see, e.g., [1,2]). Therefore the symmetry of the system is broken spontaneously and besides phonons the existence of soliton-type excitations (kinks) is possible [3-6]. The lattice distortion at the n-th site has the form:

$$s_n = (-1)^n s_0 \phi_n, \quad \phi_n = \phi(n) = \mathrm{th}\frac{n a}{\xi_0 \sqrt{2}}, \tag{1}$$

where s_0 is the distortion due to the dimerization; a, the lattice constant; and ξ_0, the soliton width. The corresponding solitons are amplitude solitons contrary to the phase solitons which are usually used to describe transitions in incommensurate structures and charge-density-waves behavior. The effective Hamiltonian of the system described by distortions s_n corresponds to the lattice scalar ϕ^4-model.

The energy of the chain with a soliton is enhanced by a soliton energy E_s and thus the appearance of solitons in the ground state is not profitable. But in the presence of donor or acceptor impurities the excess electrons or holes can lead to the creation of charged ($\pm e$) solitons if $E_s < \Delta$, where Δ is a half-width of the electronic spectrum gap in the dimerized state [3,7]. In such a way the soliton lattice is formed which can be shifted along the chain without any cost of energy thus forming a conducting state of the system.

Bak and Pokrovsky [5] have proposed the mechanism of the transition to such conducting state according to which the transition takes place when at some critical concentration of excess electrons (solitons), c_{cr}, the soliton-interaction energy becomes equal to the energy of soliton pinning to the lattice. However a more intensive pinning effect is caused by structural defects among which at least dopant impurities should be taken into account as they lead to the soliton creation. Different aspects of charge-density-waves pinning to defects were considered in many papers (see, e.g., [1,3,6-8]).

In this paper we investigate the influence of impurities on amplitude-soliton properties in one-dimensional ϕ^4-model of

Peierls systems with nearly half-filled bands. In Sec.2 the soliton-solution change near the impurity is studied with the help of the perturbation theory. Two types of impurities are considered: symmetry-conserving and symmetry-breaking impurities. The soliton lattice is investigated in Sec.3. The kink-impurity binding energy and a critical concentration at which kinks form an unpinned conducting lattice are calculated. A limiting velocity of soliton passing over the impurity is obtained and estimation of depinning temperature is given.

2. IMPURITY INFLUENCE ON A KINK

When the concentration of impurities is small one can consider them as isolated. Thus in this section we will investigate the problem of one impurity assuming hereafter the additive contribution of impurities with concentration p.

We write the model Hamiltonian in the continuum limit and in dimensionless variables in the form:

$$H = \int_{-\infty}^{\infty} dx \left(\frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 - \frac{\phi^2}{2} + \frac{\phi^4}{4} + \frac{1}{2}V(x)(\phi-\phi_d)^2\right). \quad (2)$$

The interaction of kinks with the impurity can be described by the attractive short-range potential:

$$V(x) = a\delta(x - x_p), \quad (3)$$

where x_p is the impurity coordinate. In the case of conserving-symmetry impurity (defect) its equilibrium position is defined by $\phi_d(x_p) \equiv \phi_d = 0$. In the critical phenomena approach one connects this type defect with the "random bond" or the "random temperature" problem [9]. In the case of breaking-symmetry defects the equilibrium position is different from zero ($\phi_d \neq 0$). This corresponds to the presence of a random field in the system. Note that in the case of breaking-symmetry defects there take place both a "random field" and a "random bond".

The equation of motion for displacive fields has the form:

$$\ddot{\phi} - \phi'' - \phi + \phi^3 + \gamma\dot{\phi} = -V(x)(\phi - \phi_d). \quad (4)$$

The damping constant γ describes phenomenologically the stohastic character of kink motion between their collisions.

To describe the kink-defect interaction let us represent a displacement $\phi(x)$ as a sum of an equilibrium position $\phi_0(x)$ and a fluctuation $u(x,t)$:

$$\phi(x,t) = \phi_0(x) + u(x,t). \quad (5)$$

The function $\phi_0(x)$ is the stationary partial solution of the homogeneous Eq.(4) and has the form (1). Replacing in Eq.(1) the variable na/ξ_0 by x we write:

$$\phi_0(x) = \mathrm{th}\frac{x}{\sqrt{2}}. \quad (6)$$

Substitute now Eq.(5) into Eq.(4) and obtain the equation for $u(x,t)$ in the linear approximation:

$$\ddot{u} - u'' + \left(2 - 3\,\mathrm{ch}^{-2}\frac{x}{\sqrt{2}}\right)u + \gamma\dot{u} = -V(x)u - V(x)(\phi_0 - \phi_d). \quad (7)$$

In order to solve Eq.(7) we use the complete orthonormal set $\{\Psi\}$ of eigenfunctions of the self-adjoint linear operator L:

$$L\Psi \equiv -\Psi'' + \left[2 - 3\,\mathrm{ch}^{-2}\frac{x}{\sqrt{2}}\right]\Psi = \omega^2\Psi. \quad (8)$$

The normalized solutions of this equation have the form:

$$\Psi_0(x) = \sqrt{\frac{3}{4\sqrt{2}}}\,\mathrm{ch}^{-2}\frac{x}{\sqrt{2}}, \quad \omega_0^2 = 0, \quad (9a)$$

$$\Psi_1(x) = \sqrt{\frac{3}{2\sqrt{2}}}\,\mathrm{th}\frac{x}{\sqrt{2}}\,\mathrm{ch}^{-1}\frac{x}{\sqrt{2}}, \quad \omega_1^2 = \frac{3}{2}, \quad (9b)$$

$$\Psi_k(x) = e^{ikx/\sqrt{2}}\frac{[3\,\mathrm{th}^2(x/\sqrt{2}) - 3ik\,\mathrm{th}(x/\sqrt{2}) - (1+k^2)]}{(2\pi(1+k^2)(4+k^2))^{1/2}}, \quad \omega_k^2 = 2 + \frac{k^2}{2}. \quad (9c)$$

Then the displacement $u(x,t)$ is defined by the expansion:

$$u(x,t) = \beta_0(t)\Psi_0(x) + \beta_1(t)\Psi_1(x) + \int_{-\infty}^{\infty} dk\,\beta_k(t)\psi_k(x). \quad (10)$$

Substituting Eq.(10) into Eq.(7) and using Eq.(8) and the orthonormal properties of the basis (9) we obtain the system of equations for coefficients $\{\beta\}$:

$$\ddot{\beta}_0 + \gamma\dot{\beta}_0 + (\omega_0^2 + A_{00})\beta_0 + A_{01}\beta_1 + \int_{-\infty}^{\infty} dq\,\beta_q A_{0q} = -\Delta_0 + D_0\phi_d, \quad (11a)$$

$$\ddot{\beta}_1 + \gamma\dot{\beta}_1 + (\omega_1^2 + A_{11})\beta_1 + A_{10}\beta_0 + \int_{-\infty}^{\infty} dq\,\beta_q A_{1q} = -\Delta_1 + D_1\phi_d, \quad (11b)$$

$$\ddot{\beta}_k + \gamma\dot{\beta}_k + \omega_k^2\beta_k + A_{k0}\beta_0 + A_{k1}\beta_1 + \int_{-\infty}^{\infty} dq\,\beta_q A_{kq} = -\Delta_k + D_k\phi_d, \quad (11c)$$

where

$$A_{js} \equiv \int_{-\infty}^{\infty} dx\,V(x)\Psi_j^*\Psi_s, \quad (12)$$

$$D_j \equiv \int_{-\infty}^{\infty} dx\, V(x)\, \Psi_j^* , \tag{13}$$

$$\Delta_j \equiv \int_{-\infty}^{\infty} dx\, V(x)\, \phi_0 \Psi_j^* , \quad (j, s = 0,1,k) . \tag{14}$$

The partial solution of the system of the inhomogeneous equations (11) one findes by using Fourier-transformation of $\beta_j(r)$. Then in the weak kink-defect-interaction approximation ($\alpha < 1$) we yield:

$$\beta_j^{(1)}(\omega) = -2\pi(\Delta_j - D_j\, \phi_d)\delta(\omega) G_j(\omega), \tag{15}$$

where

$$G_0(\omega) = [E_0(\omega) - \frac{A_{10}A_{10}}{E_1(\omega)}]^{-1} , \tag{16a}$$

$$G_1(\omega) = [E_1(\omega) - \frac{A_{10}A_{10}}{E_0(\omega)}]^{-1} , \tag{16b}$$

$$G_k(\omega) = E_k^{-1}(\omega), \tag{16c}$$

$$E_j(\omega) = -\omega^2 - i\gamma\omega + \omega_j^2 + A_{jj} , \quad j = 0,1, \tag{17a}$$

$$E_k(\omega) = -\omega^2 - i\gamma\omega + \omega_k^2 . \tag{17b}$$

In Eqs.(15)-(17) ω_j are the eigenvalues in Eqs.(9) and the matrix elements after calculations according to Eqs.(12)-(14) with the help of Eq.(9) have the form:

$$\Delta_0 = -\sqrt{\frac{3\sqrt{2}}{8}}\alpha \,\mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}\, \mathrm{ch}^{-2}\frac{x_0 - x_p}{\sqrt{2}} , \tag{18a}$$

$$\Delta_1 = \frac{\sqrt{3\sqrt{2}}}{2}\alpha\, \mathrm{th}^2\frac{x_0 - x_p}{\sqrt{2}}\, \mathrm{ch}^{-1}\frac{x_0 - x_p}{\sqrt{2}} , \tag{18b}$$

$$\Delta_k = -\alpha\, \mathrm{th}\frac{x_0 - x_p}{\sqrt{2}} \Psi_k^*(x_0 - x_p) , \tag{18c}$$

$$D_0 = \sqrt{\frac{3\sqrt{2}}{8}}\alpha\, \mathrm{ch}^{-2}\frac{x_0 - x_p}{\sqrt{2}} , \tag{19a}$$

$$D_1 = -\frac{\sqrt{3\sqrt{2}}}{2}\alpha\, \mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}\, \mathrm{ch}^{-1}\frac{x_0 - x_p}{\sqrt{2}} , \tag{19b}$$

$$D_k = \alpha \Psi_k^*(x_0 - x_p) , \tag{19c}$$

$$A_{00} = \frac{3\sqrt{2}}{8}\alpha\, \mathrm{ch}^{-4}\frac{x_0 - x_p}{\sqrt{2}} , \tag{20a}$$

$$A_{11} = \frac{3\sqrt{2}}{4}\alpha\, \mathrm{th}^2\frac{x_0 - x_p}{\sqrt{2}}\, \mathrm{ch}^{-2}\frac{x_0 - x_p}{\sqrt{2}} , \tag{20b}$$

$$A_{kk} = \frac{\alpha[9\,\mathrm{th}^4\frac{x_0 - x_p}{\sqrt{2}} - (6 - 3k^2)\,\mathrm{th}^2\frac{x_0 - x_p}{\sqrt{2}} + (1 + k^2)^2]}{2\pi(1 + k^2)(4 + k^2)} , \tag{20c}$$

$$A_{01} = -\frac{3\alpha}{4}\,\mathrm{sh}\frac{x_0 - x_p}{\sqrt{2}}\, \mathrm{ch}^{-4}\frac{x_0 - x_p}{\sqrt{2}} , \tag{20d}$$

where x_0 is the initial kink's position.
Futher, using Eq.(15) we obtain:

$$\beta_j^{(1)}(r) = -(\Delta_j - D_j\, \phi_d) G_j(0) . \tag{21}$$

The general solution of the system of homogeneous equations (11) one finds for small α and the weak damping constant ($\gamma < \alpha$):

$$\beta_j^{(0)}(t) = C_{1j}\, e^{-\gamma t/2} \cos\Omega_j t + C_{2j}\, e^{-\gamma t/2} \sin\Omega_j t , \tag{22}$$

where

$$\Omega_j^2 = \omega_j^2 + A_{jj} - \frac{\gamma^2}{4}, \; j = 0,1, \quad \Omega_k^2 = \omega_k^2 - \frac{\gamma^2}{4} , \tag{23}$$

and C_{j1}, C_{j2} are integration constants.

The general solution of the system of inhomogeneous equations (11) has the form:

$$\beta_j(t) = \beta_j^{(0)}(t) + \beta_j^{(1)}(t) . \tag{24}$$

Integration constants can be found from the condition of kink localization at $t = 0$: $\beta_j(0) = \dot{\beta}_j(0) = 0$. In this case using Eq.(24) together with Eqs.(21), (22) and taking into account Eqs.(16)-(20) in linear approximation in α we obtain the final expressions for $\beta_j(t)$:

$$\beta_j(t) = \beta_j^{\circ}[1 - e^{-\gamma t/2}(\cos\Omega_j t + \frac{\gamma}{2\Omega_j}\sin\Omega_j t)], \tag{25}$$

where

$$\beta_0^o = 2\sqrt{\frac{\sqrt{2}}{3}}[\phi_d + \mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}]\,\mathrm{ch}^2\frac{x_0 - x_p}{\sqrt{2}}, \tag{26a}$$

$$\beta_1^o = -\alpha\frac{\sqrt{3\sqrt{2}}}{2(\omega_f^2 + A_{11})}[\phi_d + \mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}]\frac{\mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}}{\mathrm{ch}\frac{x_0 - x_p}{\sqrt{2}}}, \tag{26b}$$

$$\beta_k^o = \alpha\frac{\Psi_k^*(x_0 - x_p)}{\omega_k^2}[\phi_d + \mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}]. \tag{26c}$$

Finally, to calculate $u(x,t)$ it is necessery to use the integral:

$$\int_{-\infty}^{\infty} dx\beta_k^o\Psi_k^*(x_0 - x_p) = \frac{5\alpha}{16}[\phi_d + \mathrm{th}\frac{x_0 - x_p}{\sqrt{2}}] \times \\ \times [1 - \frac{2}{5}\mathrm{th}^2\frac{x_0 - x_p}{\sqrt{2}} + \mathrm{th}^4\frac{x_0 - x_p}{\sqrt{2}}]. \tag{27}$$

Now the solution of the Eq.(4) can be obtained. It is defined by Eqs.(5), (6) and (10) in that using Eqs.(25)-(27). The solution (5) does show the kink changes as a result of its interaction with the impurity.

3. PINNING OF KINKS TO DEFECTS AND TO THE LATTICE

Let us consider conditions of kink's pinning to the impurity. The binding energy of a kink with the impurity is the energy difference between two configurations [8]:

$$-|E_B| = E_d - E_\infty = E_k(x_0 \to x_p) - E_k(x_0 \to x_\infty), \tag{28}$$

where

$$E_k(x_p) = \frac{1}{T}\int_0^T dt\int_{-\infty}^{x_p} 2H[\phi(x,t)]dx. \tag{29}$$

By using Eq.(5) and Eq.(2), without kinetic energy, and performing integration in Eq.(29) we find:

$$E_B = \alpha\frac{\xi_0}{a}2[1 + \frac{64 - 13\sqrt{2}}{32}\phi_d]. \tag{30}$$

In general, the solution to (2) is a soliton lattice. The soliton interaction energy can be derived by expanding the energy of the soliton lattice in small soliton concentration c (or for $\xi_0 \gg a$) [5, 12]:

$$E_{int} = NcE_0C_1\exp(-a/c\sqrt{2}\xi_0), \tag{31}$$

where C_1 is a constant (according to [12] $C_1 = 4$) and $E_0 = 8\sqrt{2}\,\xi_0/3a$ is kink energy.

Besides defects the discretness of the lattice can hinder to the movement of the soliton lattice [5, 13]. According to [5] the pinning energy of kinks to the lattice is equal to

$$E_\ell = Nc\frac{16\pi^4}{3}(\frac{\sqrt{2}\xi_0}{a})^4\exp(-\frac{\pi^2\sqrt{2}\xi_0}{a}) \tag{32}$$

for $\xi_0 \gg a$.

When concentration of impurities is small they are isolated (noninteracting) and the corresponding pinning energy of kinks, according to Eq.(30) is given by:

$$E_d \simeq Np\alpha\frac{\xi_0}{a}2[1 + \frac{64 - 13\sqrt{2}}{32}\phi_d], \tag{33}$$

where p is the impurity concentration. A critical soliton concentration c_{cr} is defined by the condition:

$$E_{int} = E_\ell + E_d. \tag{34}$$

At $c < c_{cr}$ the soliton lattice is pinned, while at $c > c_{cr}$ it can be shifted along the chain without any cost of energy. When only dopant defects are present in the system the soliton concentration c (the concentration of excess electrons) is equal to the impurity concentration p and from the condition (34) one obtains:

$$c_{cr} = \frac{a}{\sqrt{2}\xi_0}\ln^{-1}[\pi^4\sqrt{2}(\frac{\xi_0}{a})^3 e^{-\pi^2\sqrt{2}\xi_0/a} + \frac{3\sqrt{2}}{64}\alpha V(\phi_d)], \tag{35}$$

where $V(\phi_d) = 2(1 + \frac{64 - 13\sqrt{2}}{32}\phi_d)$. In absence of impurities ($\alpha = 0$) and at $\xi_0/a \gg 1$ Eq.(35) goes over to the expression for c_{cr}: $c_{cr} = a^2/2\pi^2\xi_0^2$ which was obtained in the case of lattice pinning only [5].

In Fig.1 the dependence of c_{cr} on the dimensionless kink width $y = \xi_0/a$ is shown for breaking symmetry defects ($\phi_d = 1$). For comparison we perform calculations with Eq.(35) for different

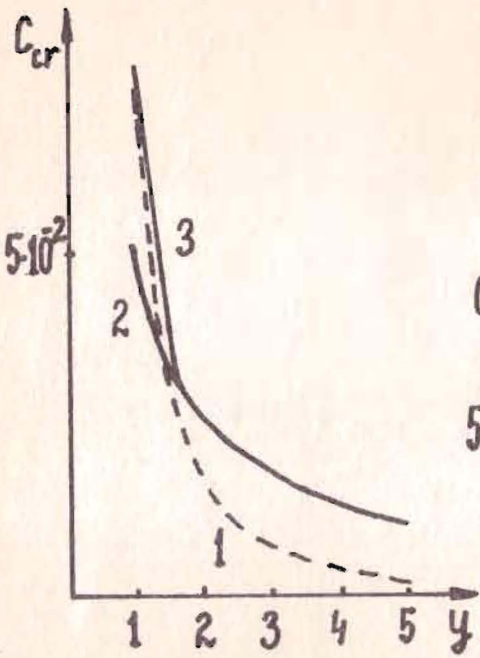

Fig.1. The soliton critical concentration c_{cr} as a function of $y = \xi_0/a$ for breaking-symmetry impurities ($\phi_d = 1$). Curves 1, 2 and 3 correspond to the pinning to the lattice, to defects and both to the lattice and defects, respectively.

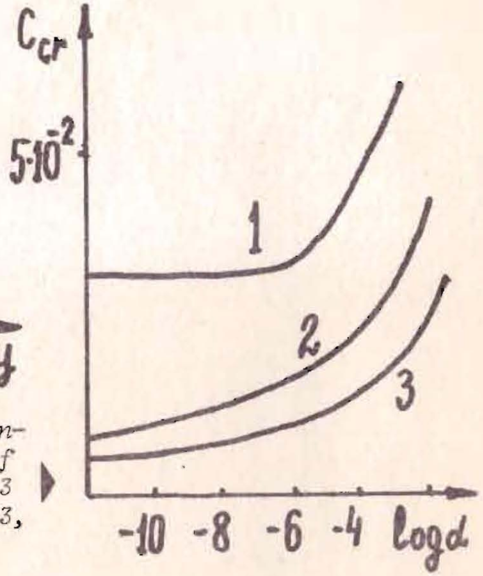

Fig.2. The soliton critical concentration c_{cr} as a function of coupling constant α at $y=1.5$, 3 and 5 for the curves 1, 2 and 3, respectively.

mechanisms of pinning: 1) only to the lattice ($\alpha = 0$), 2) only to defects ($\alpha = 10^{-5}$) and 3) to both the lattice and defects (α have the same values as in previous case). As one can see the critical concentration and the contributions of different pinning mechanisms depend crucially on the kink width. The pinning to the lattice takes place only at small values of y, while at $y \geq 2$ the essential contribution to the pinning comes from impurities. In Fig.2 the dependence of c_{cr} on the coupling constant α for $y = 1.5$, 3, and 5 is shown. The pinning of kinks to breaking symmetry impurities is stronger than to conserving symmetry ones and increases proportionally to ϕ_d.

So far we were considering the system at zero temperature. The enhancement of the temperature must lead to the depinning of kinks. Let us estimate a depinning temperature by using the relation $\theta = m_k v_k^2$, where m_k is a kink mass and v_k it's velocity. By performing the Lorenz-transformation in Eq.(6) we obtain

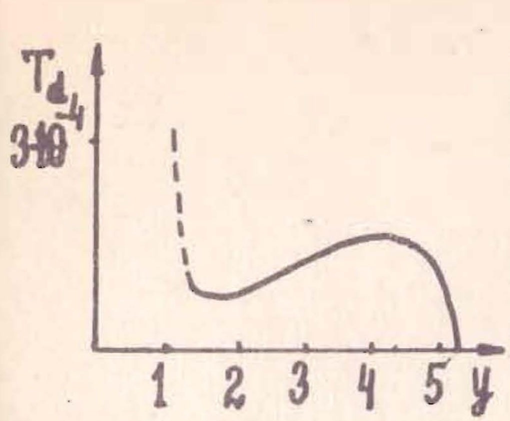

Fig.3. The depinning temperature T_d as a function of y at $c = 10^{-2}$, $\alpha = 10^{-5}$, $\phi_d = 0$.

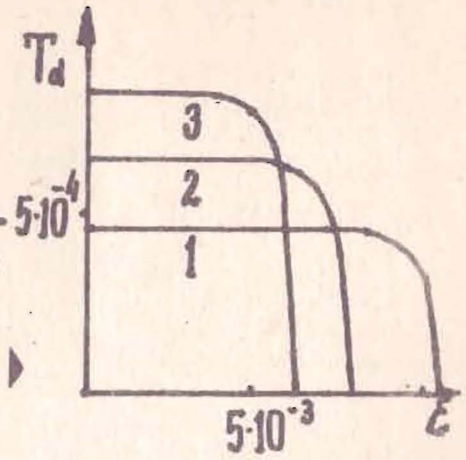

Fig.4. The dependence of depinning temperature on concentration c at $\phi_d = 1$, $\alpha = 10^{-5}$ and for y = 5, 7, 9 for the curves 1, 2, 3, respectively.

the kinetic kink energy:

$$E_k = E_k^m v_k^2 = \frac{m_k c_0^2}{8V_0}\tilde{v}_k^2 . \tag{36}$$

Here E_k^m is the maximal kinetic energy; c_0, the limiting kink velocity (the sound velocity in the medium); $V_0 = A^2/4B$ is the depth of the one-partical potential; the kink mass is $m_k = 2\sqrt{2}\,mA/3B\xi_0\, a$, being the partical mass, A/B is the squared distance between minima in the one-particle potential.

From the condition $E_k = E_B$ one can obtain the expression for the limiting velocity of a kink as passing through a defect:

$$\tilde{v}_{k,0}^2 = \alpha\, \frac{\xi_0}{a}\, \frac{4V_0}{E_k^m} 2\left[1 + \frac{64-13\sqrt{2}}{32}\phi_d\right] . \tag{37}$$

When $\tilde{v}_k < \tilde{v}_{k,0}$ a kink stopes (pinns) on a defect. From Eq.(37) it follows that the limiting velocity in the case of conserving-symmetry defects ($\tilde{v}_{k,0}^{(1)}$) and breaking-symmetry one ($\tilde{v}_{k,0}^{(2)}$) are connected by the ratio: $\tilde{v}_{k,0}^{(2)} / \tilde{v}_{k,0}^{(1)} = 1 + \frac{64-13\sqrt{2}}{32}\phi_d$. It means that in the later case a kink must have a larger kinetic energy as to pass through a defect.

The depinning temperature $T_d = \theta_d/V_0$ can be found from the condition: $T_d = 2(E_\ell + E_d - E_{int})/Nc$ if $c < c_{cr}$. Then by using Eq's.(31)-(33) we obtain:

$$T_d = \frac{32\pi^4}{3}\left(\frac{\sqrt{2}\xi_0}{a}\right)^4 e^{-\pi^2\sqrt{2}\xi_0/a} + 2\alpha\frac{\xi_0}{a}V(\phi_d) - \frac{64\sqrt{2}}{3}\frac{\xi_0}{a} e^{-a/\sqrt{2}c\xi_0}. \tag{38}$$

In fig.3 the y-dependence of T_d at $c = 10^{-2}$ is shown for different pinning mechanisms. In Fig.4 the c-dependence of T_d at various $y = 5, 7, 9$ is shown.

4. DISCUSSION

The investigations presented show that Peierls systems with half-filled bands described by the phenomenological model (2) necessarily undergo a transition from the insulating phase to the conducting one. In the insulating phase the charged amplitude solitons are pinned to dopant impurities. This phase seems to be a stable chaotic phase having properties of spin glasses [14]: When the soliton width nearly exceeds the lattice constant the impurity pinning prevails the lattice one. The former pinning growths with increasing of the kink-impurity interaction which is characterised by both the coupling constant α and the "impurity field" ϕ_d. The transition to the conducting regular incommensurate structure at low temperatures, $T < T_d$, appears at some critical consentration of the excess electrons c_{cr} which rapidly decreases with ξ_0/a.

The transition to the conducting state (the depinning of kinks) at $c < c_{cr}$ takes place when the temperature increases up to $T \geq T_d$. An external electric field will act in the same way [5].

Our results can be applied for the qualitative description of the insulator-metal transition in trans-polyacetylene for which, as has been estimated in ref. [3,5], $2a < \xi_0 < 6a$. Of course our model of dopant impurities is oversimplified and has to be improved for a detailed comparison with experiments. In a more realistic model it is necessary to include screening effects, electronic correlations as well as electron-dopant and interchain interactions [15,16].

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в пайерлсовских системах с примесями

Исследовано влияние примесей на свойства амплитудных солитонов в одномерной модели пайерлсовских систем с почти наполовину заполненными зонами. Показано, что имеется критическая концентрация, при которой солитоны образуют незакрепленную, проводящую решетку.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1984

Aksenov V.L., Didyk A.Yu., Zakula R. E17-84-483
Pinning of Amplitude Solitons
in Peierls Systems with Impurities

The influence of impurities on properties of amplitude solitons in a one-dimensional model of Peierls systems with nearly half-filled bands is investigated. It is shown that there takes place a critical concentration at which the solitons form an unpinned conducting lattice.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1984