# Thermodynamics of soliton excitations in a system of polyacetylene chains

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A two-dimensional (2*D*) system of trans-$(\mathrm{CH})_x$ chains with weak interaction between the chains is studied in the presence of donor (acceptor) impurities. The presence of a small number of donor electrons leads to formation of solitons on the polyacetylene chains. The weak interaction between the chains produces in the system an Ising-type transition from a state in which the solitons are paired (low-temperature phase) into a state with free solitons. The effective soliton coupling energy near the phase-transition temperature is calculated. The effect of the interaction between the solitons and the impurities on the phase-transition temperature is considered. It is shown that the phase transition can be observed only if the interaction between the chains is not too weak, e.g., $J_\perp \gtrsim E_S n/\ln n^{-1}$, where $E_S$ is the soliton energy and $n$ is the chain impurity density. Otherwise, interaction between solitons and impurities causes vanishing of the phase transition. The results are qualitatively extended to include the case of a real three-dimensional system.

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## 1. INTRODUCTION

It is known the Peierls instability due to the electron-phonon interaction makes the ground state of the *trans*-$(\mathrm{CH})_x$ chain doubly degenerate (Fig. 1). Systems of this type have been under study for quite a while (see, e.g., Ref. 1). In the ground state the symmetry between the " + " and " − " states (see Fig. 1) is spontaneously broken, and in addition to phonons the system admits of formation of excitations such as solitons, which are chain deformations that describe a smooth transition from the " + " to " − " state and vice versa. The properties of such soliton excitations were investigated in detail[2,4] for isolated polyacetylene chains.

The energy of a chain with a soliton increases by approximately $E_S = 0.6\Delta$, where $2\Delta = 1.4$ eV is the width of the gap in the electron spectrum. One state for each spin orientation is produced in the electron spectrum at the center of the forbidden band. Each such state was made up of half a state for one valence-band spin and half a state for one conduction-band spin. Depending on the number of electrons localized on the soliton (0, 1, or 2) the soliton can have a charge $+e$, 0, and $-e$ with respective spin zero, 1/2, and zero.[2] From the condition that the number of electrons and the total spin be conserved it follows that solitons can be produced only in pairs. Accordingly only an integer number of states can leave the valence or conduction band.

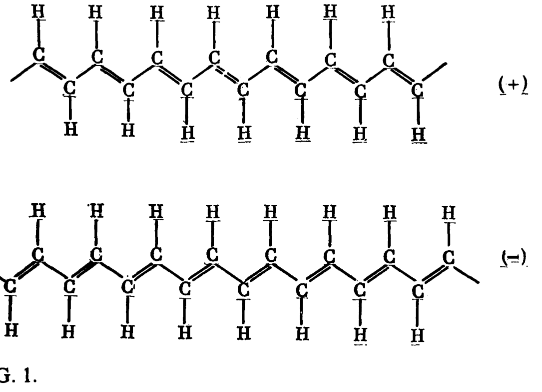

FIG. 1.

Since $E_S < \Delta$, charged solitons are produced on the chains when a small number of donor (acceptor) impurities is added to the system.[5] Because of the solitons, the donor electrons (holes) form a narrow band at the center of the forbidden band, and do not fill the lower part of the conduction band (Fig. 2). Thus, the number of solitons on the acetylene chain is determined by the number of donor (acceptor) impurities.

A large number of experiments confirm the existence of mobile paramagnetic defects (uncharged spin-processing domain walls—solitons) in pure polyacetylene.[6–8] It has also been shown that a strong increase of the polyacetylene conductivity by donor impurities takes place without a corresponding increase of the spin susceptibility,[9] and that the localized states produced by light doping are nonmagnetic.[10] This means that the mobile charges produced by light doping of *trans*-$(\mathrm{CH})_x$ are indeed charged spinless solitons.

Up to now, the properties of solitons in polyacetylene were theoretically analyzed without allowance for the interaction between the chains, although actually even a weak interchain interaction can influence strongly the thermodynamic properties of a soliton system. In Ref. 11 was advanced the simple idea that the thermodynamics of solitons in the presence of weak interaction between the chain is described by the Ising anisotropic model (see Sec. 2). In such a system, a phase transition takes place from the low-tempera-

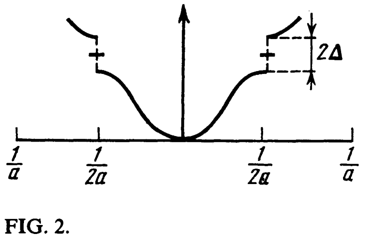

FIG. 2.

ture phase, where all the solitons on the chains are bound into pairs and a strong correlation exists at low temperatures between the pair positions on different chains (the soliton pairs are aligned into long strings), to the high-temperature phase, where all the solitons are free.[11] To obtain information on how such a phase transition can manifest itself in the observed quantities, the effective energy of the interaction between solitons bound into pairs in the low-temperature phase is calculated in Sec. 3.

For simplicity, and in view of the possibility of obtaining exact results, we consider a two-dimensional system of polyacetylene chains. The qualitative conclusions can then be easily generalized to include the three-dimensional case.

For a two-dimensional system one can also examine how the interaction of solitons with the impurities (to which these solitons owe their existence) influences the temperature of the phase transition (Sec. 4). The interaction of solitons with impurities can be described by introducing impurity bonds into the corresponding Ising model. Using the methods developed for the two-dimensional Ising model,[12] one can calculate to first order in the impurity density the shift of the transition temperature. This correction yields an estimate of the magnitude of the interaction between the chains and of the impurity density at which the phase transition in the system can vanish, i.e., the solitons become localized on the impurities and the system is in a "paramagnetic" state at all temperatures. It will be shown that the phase transition described in Ref. 11 can occur only if the energy of the interaction between the chains $J_\perp \gtrsim \Delta n/\ln n^{-1}$, where $n$ is the impurity density.

## 2. THE MODEL

So long as the polyacetylene chains do not interact, there is also practically no interaction between the solitons in the chains, inasmuch as the elastic strains fall off exponentially far from the solitons. Assume now a weak interaction between the chains, which manifests itself in the fact that the states on the neighboring chains "+ +" and "+ −" have different energy. We consider a planar (two-dimensional) system of parallel chains with nearest-neighbor interaction. Then, if a soliton and antisoliton on some chain are separated by a distance $R$ (Fig. 3), the state of this system will be $2J_\parallel + RJ_\perp$, where $J_\parallel \equiv E_S$ is the soliton energy, and $J_\perp$ is the chain-interaction energy per unit length. We shall not take into account here the fact that the soliton has a finite size, actually about seven lattice periods, since this does not change the qualitative picture. We take this size to be the minimum linear dimension and regard it as the unit length.

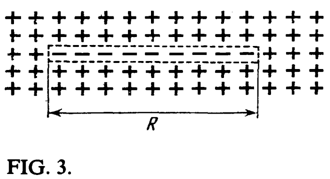

FIG. 3.

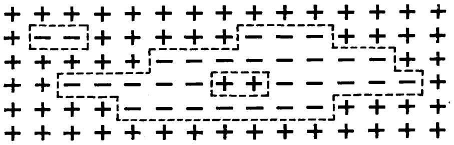

FIG. 4.

In the general case, when the segments between solitons on neighboring chains overlap (Fig. 4), the energy is $L_\parallel J_\parallel + L_\perp J_\perp$, where $L_\parallel$ and $L_\perp$ are the total lengths of the vertical and horizontal sections of the contour that surrounds the region inside the solitons. We see thus that the thermodynamics of such soliton excitations is described by the anisotropic Ising model with Hamiltonian

$$H_0 = -\beta \sum_x (J_\parallel \sigma_x \sigma_{x+\hat{1}} + J_\perp \sigma_x \sigma_{x+\hat{2}}), \tag{1}$$

where the variables $\sigma$, which take on values $\pm 1$, are specified at the sites of the square lattice, and $\hat{1}$ and $\hat{2}$ are unit orthogonal vectors (the vector $\hat{1}$ indicates the direction of the chains). In our problem, however, there is a supplementary condition that fixes the soliton density on the chains. This condition can be easily taken into account by introducing into the Hamiltonian (1) the chemical potential $\mu$:

$$H_0 \to H = -\beta \sum_x [(J_\parallel + \mu) \sigma_x \sigma_{x+\hat{1}} + J_\perp \sigma_x \sigma_{x+\hat{2}}] \tag{2}$$

and stipulating that

$$\partial F/\partial \mu = n, \tag{3}$$

where $n$ is the linear density of the donor impurities and $F$ is the free energy:

$$F = -\ln Z, \tag{4}$$

$$Z = \sum_{\{\sigma\} = \pm 1} \exp\{-H\}. \tag{5}$$

If we disregard the interaction of the solitons with the impurities (i.e., assume that $J_\parallel$ is independent of the coordinates), we can calculate in standard fashion (see, e.g., Ref. 13) the free energy (4), (5). Solving next the condition (3) with respect to $(J_\parallel + \mu)$ or $J_\perp$ and substituting the result in the free energy, we can determine the transition temperature. This was done in Ref. 11, with the result

$$T_c \approx (2/\pi)(J_\perp/n) \tag{6}$$

(in first order in $n \ll 1$). This result means that for this analysis to be valid it is necessary that the interaction $J_\perp$ between the chain be at any rate small compared with $n\Delta$.

The phase transition proceeds in the following manner. At low temperatures all the solitons on the chains are paired, and the positions of the pairs on different chains are so correlated that the pairs are next to one another and form strings of length $n \exp(-J_\perp/n)$ across the chains.[11] The reason is that the soliton density, or the density of the "excited" Ising bonds $J_\parallel$, is fixed and equal to $n$, whereas the density of the excited bonds $J_\perp$ is controlled by the temperature, is equal to $\exp(-J_\perp/n)$, and determines the number of strings in the system. With increasing temperature the strings become shorter, vanishing at $T^* \sim J_\perp/\ln n^{-1}$, but the solitons on the chains remain paired as before. For soliton pairs to break, the pair dimension must become of the order of $n^{-1}$, hence the result (6).

Notice must be taken here, however, of the following circumstance. According to Ref. 2, the soliton has a rather small mass, $M_S \approx 6m_e$. Therefore the classical approach described above is valid only if the temperatures are not too low. Since the soliton and antisoliton interact in accord with the law

$$U(R) \propto J_\perp R, \tag{7}$$

the classical approach is applicable when the pair energy is much larger than the level spacing $\sim \hbar J_\perp (2M_S E)^{-1/2}$, i.e., $E \gg (\hbar^2 J_\perp^2 / 2M_S)^{1/3}$. Let

$$J_\perp = k(\Delta/a), \tag{8}$$

where $\Delta \approx 1.4$ eV, $a \approx 1.22$ Å is the period of the polyacetylene chain, and $k$ is a small parameter that determines the smallness of the distance between the chains. The validity of the classical approach is then defined by the condition

$$T \gg T_0 \approx 2{,}7 \cdot 10^2 k^{2/3} \Delta. \tag{9}$$

From the conditions $T_0 \ll T_c \sim k\Delta/n$ and $T_c \ll \Delta$ we obtain conditions on $n$ and $k$:

$$k \ll n \ll 10^2 k^{1/3}. \tag{10}$$

We note in this connection that the strings referred to above are certainly in the quantum region (the distance between the solitons and the pairs making up a string is of the order of the soliton size) so that the extent to which the estimates of their number and sizes are correct is actually unclear.

### 3. EFFECTIVE SOLITON-INTERACTION ENERGY

Near the phase-transition point, the dimension of the soliton pair on a chain becomes large, so that the influence of solitons located on neighboring chains becomes important. Therefore the effective soliton-antisoliton pair energy, which should be equal to (7) far from the transition point, is renormalized. To understand how the phase transition takes place, we turn first to the general equations (2)–(5).

The free energy (4), (5) of the Ising system (2) can be calculated by the well-known standard methods of the Ising-model theory, and there is no need to repeat them here. The calculations are given in concise form in the Appendices. The reader interested in the details of these calculations can find them, e.g., in Refs. 13 and 14.

The result for the free energy is of the form (Appendix A)

$$F = -\int_{-\pi}^{\pi} \frac{dp_1\,dp_2}{(2\pi)^2} \ln\left[m^2 + 4\lambda_1(1-\lambda_2^2)\sin^2\frac{p_1}{2} + 4\lambda_2(1-\lambda_1^2)\sin^2\frac{p_2}{2}\right], \tag{11}$$

where

$$\lambda_1 = \operatorname{th} \beta(J_\parallel + \mu), \quad \lambda_2 = \operatorname{th}(\beta J_\perp). \tag{12}$$

A phase transition occurs when the "mass"

$$m = 1 - \lambda_1 - \lambda_2 - \lambda_1\lambda_2 \tag{13}$$

vanishes. Condition (3) can be written in the form

$$G^{*22}(0) \equiv \int_{-\pi}^{\pi} \frac{dp_1\,dp_2}{(2\pi)^2}\left[(1-\lambda_1^*)m + i\lambda_2^*(1-\lambda_1^{*2})\sin p_2 + 4\lambda_1^*\sin^2\frac{p_1}{2} + 2\lambda_2^*(1-\lambda_1^{*2})\sin^2\frac{p_2}{2}\right]\left[m^2 + 4\lambda_1^*(1-\lambda_2^{*2})\sin^2 p_1/2 + 4\lambda_2^*(1-\lambda_1^{*2})\sin^2\frac{p_2}{2}\right]^{-1} = 1-n, \tag{14}$$

$$\lambda_1^* = e^{-2\beta J_\perp}, \quad \lambda_2^* = e^{-2\beta(J_\parallel+\mu)}. \tag{15}$$

The solution of (14) together with the equation

$$\lambda_1 + \lambda_2 + \lambda_1\lambda_2 = 1$$

determines the phase-transition point:

$$\lambda_2^{*(c)} = \lambda_2^{(c)} \approx \pi n/2, \quad \lambda_1^{*(c)} = \lambda_1^{(c)} \approx 1 - \pi n$$

(the solutions are given here in first order in $n \ll 1$).

We note that in the language of the variables $\sigma$ a soliton (antisoliton) is a connection between two neighboring points, $\mathbf{x}$ and $\mathbf{x} + \hat{1}$, at which the spins are oppositely directed ($\sigma_x \sigma_{x+\hat{1}} = -1$), the condition (3) that the number of solitons on the chains be constant is equivalent to the condition

$$^1/_2(1 - \langle \sigma_x \sigma_{x+\hat{1}} \rangle) = n.$$

The proximity to the phase-transition point is determined by the smallness of the mass $m$. In the critical region at $m \sim \tau \equiv (T - T_c)/T \to 0$ the correlation radius increases like $r_c(\tau) \sim m^{-1}$. At distances $r \gg r_c$ the correlation in the system falls off like $\exp(-r/r_c)$, while power-law asymptotic scaling relations are realized inside the correlation radius.[15] In terms of the variables $\sigma$, ferromagnetic order sets in the system below the phase-transition point, i.e., a value $\langle \sigma \rangle \neq 0$ appears. At $\tau \ll 1$ (see, e.g., Ref. 16) we have

$$\langle \sigma \rangle \sim \tau^{1/8}. \tag{16}$$

Let us see what this means in the language of the solitons of the initial physical systems. Assume that at $T < T_c$ we have $\langle \sigma \rangle > 0$. We introduce the quantity

$$\Gamma_\pm(R) = \left\langle \frac{1 \pm \sigma_{x_0}}{2} \prod_{x=x_0}^{x_0+(R-1)\hat{1}} \left(\frac{1 + \sigma_x \sigma_{x+\hat{1}}}{2}\right) \right\rangle. \tag{17}$$

The mean value $\Gamma_\pm(R)$ is the probability of the soliton and antisoliton moving apart a distance $R$ in a way that no other solitons are produced between them, with $\Gamma_-(R)$ and $\Gamma_+(R)$ corresponding respectively to the situation wherein $\sigma = -1$ or $\sigma = +1$ on the chain between the solitons. The quantities $\Gamma_\pm(R)$ can be represented in the form

$$\Gamma_\pm(R) = {}^1/_2[\langle K(R) \rangle \pm \langle \sigma_{x_0} K(R) \rangle], \tag{18}$$

$$K(R) = \prod_{x=x_0}^{x_0+(R-1)\hat{1}} \left(\frac{1 + \sigma_x \sigma_{x+\hat{1}}}{2}\right). \tag{19}$$

Obviously, at $T > T_c$ we have $\Gamma_+ = \Gamma_- = 1/2\langle K(R) \rangle$. At $T < T_c$ the quantity $\Gamma_-(R)$ is the probability of formation, against the general ferromagnetic background $\langle \sigma \rangle > 0$, of a "kink" of length $R$ on which $\sigma = -1$, i.e., the probability that the dimension of the soliton-antisoliton pair is $R$. In this sense, the quantity

$$U(R) = -\ln \Gamma_-(R) \tag{20}$$

can be called the energy of the interaction between the soliton and the antisoliton.

As the phase-transition point is approached, there are two temperature regions:

$$1.\ \tau\sim m\gg n,\ r_c\ll n^{-1}, \tag{21}$$

$$2.\ \tau\sim m\ll n,\ r_c\gg n^{-1}. \tag{22}$$

It is easily understood that in the first case, when the correlation length is much shorter than the average distance between the solitons, the behavior of the correlator $\Gamma_-(R)$ at distances $R\gg r_c\sim m^{-1}$ is determined only by the mass:

$$\Gamma_-(R)\approx e^{-mR}, \tag{23}$$

which corresponds to linear attraction between the soliton and the antisoliton in the pair:

$$U(R)=mR\sim|\tau|R. \tag{24}$$

Thus, at temperatures not too close to the transition point ($n\ll\tau\ll 1$) the average size of the pair is $R(\tau)\sim\tau^{-1}$.

In the second case, in the immediate vicinity of the transition temperature, we find ourselves in the scaling region (at distances $R\ll r_c$). The correlators $\langle K(R)\rangle$ and $\langle\sigma K(R)\rangle$ can be calculated here by the methods used to calculate the usual correlation function $\langle\sigma_0\sigma_R\rangle$ of the Ising model at the transition point.[17] If we are interested in distances smaller than the average distance $n^{-1}$ between the solitons, the result is (Appendix B):

$$\begin{aligned}\Gamma_-(R)&\sim R^{-3/16}(1-c|\tau|^{1/8}R^{1/8}),\\ \Gamma_+(R)&\sim R^{-3/16}(1+c|\tau|^{1/8}R^{1/8}),\end{aligned} \tag{25}$$

where $c$ is a constant. At distances larger than $n^{-1}$, the correlator $\Gamma_-(R)$ begins to decrease exponentially like $\exp(-nR)$, this being a natural consequence of the conservation of the number of solitons on the chain.

Above the transition point we have

$$\Gamma_-(R)=\Gamma_+(R)\sim R^{-3/16}. \tag{26}$$

Thus, near the phase transition point ($|\tau|\ll n$) the soliton and antisoliton interact at distances $R\ll n^{-1}$ in accord with the law

$$U(R)\sim{}^3/_{16}\ln R+c|\tau|^{1/8}R^{1/8},\ T<T_c, \tag{27}$$

$$U(R)\sim{}^3/_{16}\ln R,\ T>T_c. \tag{28}$$

Therefore the energies of a soliton and antisoliton belonging to one pair (between which $\sigma=-1$) and of a soliton and antisoliton from different pairs (between which $\sigma=+1$) differ by the small quantity $\sim|\tau|^{1/8}R^{1/8}$. In this sense the solitons at temperatures $|\tau|\ll n$ are already "quasifree," and pairs as such do not exist.

Above the transition point ($T>T_c$) in the "paramagnetic" phase any two neighboring solitons interact in accord with (28).

## 4. EFFECT OF IMPURITIES

A very important question is how the phase transition described above is affected by interactions between the solitons and the impurities that give rise to them, since generally speaking[2] the energy of the interaction between a soliton and an impurity atom is of the order of the energy $E_S$ of the soliton itself.

Impurity atoms located between polyacetylene chains cause, first, the energy of the solitons on the chains, which we have designated $J_\parallel$, to become independent on the coordinates; second, the chain-interaction energy $J_\perp$ changes in the vicinity of the impurity atom. We start from the following model postulate. A soliton has a certain fixed energy $\tilde{J}_\parallel$ when located in the vicinity of an impurity atom, and an energy $J_\parallel$ outside this vicinity. We shall assume that the length of this vicinity is of the order of the soliton dimension, i.e., is equal to unity. Therefore, in the language of the Ising model, in this situation impurity bonds $\tilde{J}_\parallel$ are randomly distributed with low density $\nu$ in the system (actually, of course, $\nu\equiv n$). Accordingly, the change of the chain interaction energy is taken into account analogously, namely by introducing into the system impurity bonds of energy $\tilde{J}_\perp$.

Using the formalism developed for the Ising $2D$ model with impurity bonds,[12] we can calculate for the model described above, in first order in $\nu$, the shift of the transition temperature as a function of $\tilde{J}_\parallel$, $\tilde{J}_\perp$, $n$, and $T_c\sim J_\perp/n$. Of physical interest, of course, is not the shift itself, since all the calculations are valid only so long as it is small, but the direction relative to $T_c$ in which the shift takes place, and most importantly, under which conditions the shift of the transition temperature ceases to be small. We shall see below that in first order in $\nu$ the interaction of the solitons with the impurities always lowers the transition temperature. The result permits an estimate of the parameters $\tilde{J}_\parallel-J_\parallel$, $J_\perp$, and $n$ at which the lowering of the temperature becomes substantial and the phase transition may vanish.

To find the transition-temperature shift in first order in $\nu$ we use the method developed in Ref. 2 for the usual Ising model with impurity bonds. Following this reference, we must calculate the mass increment (13) linear in $\nu$, which appeared after averaging over the impurities. The transition temperature is determined from the condition

$$m(\nu)=0 \tag{29}$$

and from Eq. (15), which must be averaged over the impurities:

$${}^1/_2(1-\langle\overline{\sigma_x\sigma_{x+\hat{1}}}\rangle=n. \tag{30}$$

The calculations (Appendix C) yield for the transition temperature

$$\frac{J_\perp}{T_c(\nu)}\approx\frac{J_\perp}{T_c^{(0)}}+\frac{\pi}{2}\nu n\left(1-\frac{\tilde{J}_\perp}{J_\perp}\right)+\frac{\pi}{2}\nu n^2\left(\exp\left\{2\frac{J_\parallel-\tilde{J}_\parallel}{T_c^0}\right\}-1\right)^2, \tag{31}$$

where $T_c^{(0)}$ is the transition temperature in the absence of impurity bonds.

The second term in the right-hand side of (31) is due to the change, by the impurities, of the bonds between the chains $J_\perp$; this term is always small. Of greatest interest is the third term, which describes the shift of the transition temperature on account of the interaction of the solitons with the impurities. Although this term is of the order $vn^2$, the quantity $\exp\{2(J_\| - \tilde{J}_\|)/T_c^{(0)}\}$ may turn out to be large, since $J_\| - \tilde{J}_\| \sim \Delta$, and the transition temperature $T_c^{(0)} \sim J_1/n$ is certainly much less than $\Delta$. Thus, Eq. (34) yields an estimate of the soliton-impurity interaction energy $J_\| - \tilde{J}_\|$ at which a phase transition can exist:

$$(J_\| - \tilde{J}_\|) \leqslant T_c^{(0)} \ln n^{-1}. \tag{32}$$

In the opposite case the solitons become simply localized on the impurities and, of course, there is no phase transition at all. Estimates[2] show that $(J_\| - \tilde{J}_\|) \sim \Delta$. Since $T_c^{(0)} \approx J_\perp/n$, the phase transition described in Ref. 11 and in Sec. 2 can be observed only if the impurity density is low enough and the interaction between the chains is not too weak:

$$J_\perp/n \gtrsim \Delta/\ln n^{-1}. \tag{33}$$

## CONCLUSION

We have considered a two-dimensional system of polyacetylene chains with weak coupling between the chains and a low density of donor (acceptor) impurities. We have seen that under certain conditions a phase transition should take place in such a system from a state in which all the solitons on the chains are connected in pairs (at low temperatures) into a state in which the solitons on the chains are free. To find out how this phase transition manifests itself in observable quantities, we calculated the temperature dependence of the effective interaction energy of solitons in pairs in the low-temperature phase near the phase-transition point (24), (27). We have also determined when the interaction between the solitons and the impurities that generate them is significant and can destroy the phase transition.

The calculations were performed for a $2D$ model system, for it is precisely in this case, by using the formalism of the Ising $2D$ model, that certain accurate results can be obtained and a general picture of the phase transition can be obtained.

Certain qualitative generalizations can be easily made to include the case of a real three-dimensional system with interaction between the chains. It is clear that in this case a similar phase transition, described by the Ising $3D$ model, takes place at a temperature $T_c \sim J_\perp/n$. In the low temperature phase the solitons are bound into pairs. As the phase-transition is approached, the size of the soliton pairs on the chains increases[15] like $r_c(\tau) \sim \tau^{-\nu} (\nu \approx 0.63)$; in this case $r_c(\tau) \ll n^{-1}$, where $r_c$ is the correlation radius of the Ising $3D$ model. Under these conditions the soliton and the antisoliton in the pair are bound by an effective potential $U(R) \sim r_c^{-1}(\tau) R$. In the immediate vicinity of the transition point, where $r_c(\tau) \gg n^{-1}$, an interaction similar to (27) takes place and is of the form

$$U(R) \sim \zeta_{3D} \ln R + \text{const}\, |\tau|^\beta R^\beta,$$

where $\beta \approx 0.34$ and $\zeta_{3D}$ is a certain universal critical index.

It is much more difficult to take into account the effect of the interaction between the solitons and the impurities in the three-dimensional case, for to calculate the temperature account must be taken of the local lattice degrees of freedom, i.e., to find the shift of the transition temperature [an equation similar to (31)] we need at least an exact solution of the Ising $3D$ model. Nonetheless, the estimate (33) for the parameters $J_\perp$ and $n$ at which a phase transition is possible remains valid also in the three-dimensional case, since this estimate is a consequence of simply the fact that any correction to the transition temperature $T_c \sim J_\perp/n$ is of the form

$$n^k f\left[\exp\left(\frac{J_\| - \tilde{J}_\|}{T_c}\right)\right].$$

In light of the latest experiments on weakly doped polyacetylene, in which an impurity-density phase transition from the dielectric state to a metal is observed,[18] it would be of very great interest to understand how the low-temperature properties and the phase transition in weakly doped polyacetylene, described in Ref. 11 and in this paper, manifest themselves in observable quantities such as, say, the conductivity.

In conclusion the author thanks S. A. Brazovskiĭ and Tomas Bohr for numerous discussions, as well as V. L. Pokrovskiĭ and L. P. Gor'kov for a helpful discussion of the work.

## APPENDIX A

It is known that the Ising-model partition function

$$Z = \sum_{\sigma} e^{-H}, \tag{A.1}$$

where

$$H = -\beta \sum_{x,\alpha} J_{x\alpha} \sigma_x \sigma_{x+\hat{\alpha}}, \tag{A.2}$$

can be represented in equivalent form in terms of the Grassman variables $\psi_x^\alpha (\alpha = 1,2,3,4)$, specified at the sites of the $2D$ lattice, and having, by definition, the properties (see, e.g., Ref. 14):

$$\begin{gathered} \psi_x^\alpha \psi_{x'}^\beta + \psi_{x'}^\beta \psi_x^\alpha = 0, \\ \int d\psi_x^\alpha = 0, \quad \int d\psi_x^\alpha \, \psi_{x'}^\beta = \delta^{\alpha\beta} \delta_{xx'}. \end{gathered} \tag{A.3}$$

In terms of these variables, the partition function (A.2) can be written in the form[14]

$$Z = \left( \prod_x \int d\psi_x^1 \, d\psi_x^2 \, d\psi_x^3 \, d\psi_x^4 \right) e^{A[\psi]}, \tag{A.4}$$

$$A[\psi] = -{}^1/_2 \sum_x \bar{\psi}_x^\alpha \psi_x^\alpha + {}^1/_2 \sum_{x,\alpha} \lambda_{x\alpha} \bar{\psi}_{x+\hat{\alpha}}^\alpha P_\alpha^{\alpha\beta} \psi_x^\beta. \tag{A.5}$$

In the Lagrangian (A.5) we have used the notation

$$\bar{\psi}^\alpha = \psi^\beta \hat{C}^{\beta\alpha}, \quad \hat{C} = \begin{vmatrix} 0 & -1 & 1 & -1 \\ 1 & 0 & -1 & 1 \\ -1 & 1 & 0 & -1 \\ 1 & -1 & 1 & 0 \end{vmatrix},$$

$$\begin{gathered} \hat{P}_1 = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{vmatrix}, \quad \hat{P}_2 = \begin{vmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}, \\ \hat{P}_3 = \begin{vmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{vmatrix}, \quad \hat{P}_4 = \begin{vmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{vmatrix}, \end{gathered} \tag{A.6}$$

$$\lambda_{x\alpha}=\mathrm{th}(\beta J_{x\alpha}). \qquad (A.7)$$

In terms of the Lagrange theory (A.4), (A.5) we can define the Green function

$$G^{\alpha\beta}(\mathbf{x}_1\mathbf{x}_2)=\langle\bar{\psi}_{x_1}{}^{\alpha}\psi_{x_2}{}^{\beta}\rangle \qquad (A.8)$$

and verify that it satisfies the linear equation

$$G^{\alpha\beta}(\mathbf{x}_1\mathbf{x}_2)=\sum_{\gamma=1}^{4}\lambda_{x_2\beta}G^{\alpha\gamma}(\mathbf{x}_1,\mathbf{x}_2+\hat{\beta})P_{\beta}{}^{\gamma\beta}+\delta_{x_1x_2}. \qquad (A.9)$$

In the Fourier representation

$$\hat{G}(\mathbf{x}_1-\mathbf{x}_2)=\int\frac{d^2p}{(2\pi)^2}\exp\{i(\mathbf{p},\mathbf{x}_1-\mathbf{x}_2)\}\hat{G}(\mathbf{p}) \qquad (A.10)$$

this equation has a solution

$$\hat{G}(\mathbf{p})=[1-\hat{\Lambda}(\mathbf{p})]^{-1}, \qquad (A.11)$$

where $\hat{\Lambda}(\mathbf{p})$ is the so-called random-walk matrix, which in our anisotropic case, when the horizontal and vertical coupling constants are $\lambda_1=\tanh\beta(J_{\|}+\mu)$ and $\lambda_2=\tanh\beta J_{\perp}$, takes the form

$$\hat{\Lambda}(p_1p_2)=\left|\begin{array}{cccc}\lambda_1e^{ip_1} & \lambda_2e^{ip_2} & 0 & -\lambda_2e^{-ip_2}\\ \lambda_1e^{ip_1} & \lambda_2e^{ip_2} & \lambda_1e^{-ip_1} & 0\\ 0 & \lambda_2e^{ip_2} & \lambda_1e^{-ip_1} & \lambda_2e^{-ip_2}\\ -\lambda_1e^{ip_1} & 0 & \lambda_1e^{-ip_1} & \lambda_2e^{-ip_2}\end{array}\right|. \qquad (A.12)$$

The matrix (A.12) can be used to calculate the free energy of the system (see, e.g., Ref. 13)

$$F=-\ln Z=-\int_{-\pi}^{\pi}\frac{dp_1\,dp_2}{(2\pi)^2}\ln\{\det[1-\hat{\Lambda}(p_1p_2)]\}. \qquad (A.13)$$

It can be verified by direct calculation that

$$\det[1-\hat{\Lambda}(p_1,p_2)]\equiv\Delta(p_1p_2)=m^2+4\lambda_1(1-\lambda_2{}^2)\sin^2\frac{p_1}{2}+4\lambda_2(1-\lambda_1{}^2)\sin^2\frac{p_2}{2}, \qquad (A.14)$$

$$m=1-\lambda_1-\lambda_2-\lambda_1\lambda_2. \qquad (A.15)$$

At the phase-transition point $m=0$. The smallness of the mass $m$ determines the proximity in temperature to the phase-transition point: at $m\ll 1$ we have $m\sim\tau=(T-T_c)/T_c$, where $T_c$ is the transition temperature.

It is known that the Ising $2D$ model has the self-duality property (the Kramers–Wannier symmetry[19]). In terms of dual variables specified at the centers of the $2D$-lattice wafers (at the sites of the dual lattice, see, e.g., Ref. 20), the partition function of the Ising $2D$ model is given by (A.1) with the Hamiltonian (A.2), in which the following substitutions are made:

$$\begin{aligned}\lambda_1&\equiv\mathrm{th}\,\beta(J_{\|}+\mu)\to\lambda_1{}^*=e^{-2\beta J_{\perp}},\\ \lambda_2&\equiv\mathrm{th}\,\beta J_{\perp}\to\lambda_2{}^*=e^{-2\beta(J_{\|}+\mu)}.\end{aligned} \qquad (A.16)$$

Following Ref. 17, it can be easily shown that the condition (3), written in the form

$$^1/_2(1-\langle\sigma_{x+\hat{1}}\sigma_x\rangle)=n, \qquad (A.17)$$

can be represented as

$$^1/_2(1-\langle\exp\{-2\lambda_2{}^*\bar{\psi}^{\alpha}_{x+\hat{2}}P_2^{\alpha\beta}\psi_x{}^{\beta}\}\rangle)=n, \qquad (A.18)$$

where the averaging is with the aid of the Lagrangian (A.5). Expanding the exponential in (A.18) and using (A.9), we easily verify that

$$\begin{aligned}\langle\exp\{-2\lambda_2{}^*\bar{\psi}^{\alpha}_{x+\hat{2}}P_2^{\alpha\beta}\psi_x{}^{\beta}\}\rangle&=1+2\lambda_2{}^*G^{*\alpha\beta}(\mathbf{x},\mathbf{x}+\hat{2})P_2^{\alpha\beta}\\ &=1+2G^{*22}(\mathbf{x},\mathbf{x}).\end{aligned}$$

We therefore have in lieu of (A.17) the equation

$$G^{*22}(\mathbf{x},\mathbf{x})=-n. \qquad (A.19)$$

The Green function $G^{*22}(\mathbf{x},\mathbf{x})$ is a sum over all closed loops that pass through the point $\mathbf{x}$ in the $\hat{2}$ direction, and can be calculated from the relation (see Ref. 17)

$$G^{*22}(\mathbf{x},\mathbf{x})=\int_{-\pi}^{\pi}\frac{dp_1\,dp_2}{(2\pi)^2}G^{*22}(p_1,p_2)-1 \qquad (A.20)$$

(the 1 is subtracted to exclude the "zero size" loop). Direct calculation with the aid of (A.11) and (A.12) yields

$$G^{*22}(p_1,p_2)=\frac{1}{\Delta(p_1,p_2)}\Big[(1-\lambda_1{}^*)m+i\lambda_2{}^*(1-\lambda_1{}^{*2})\sin p_2+4\lambda_1{}^*\sin^2\frac{p_1}{2}+2\lambda_2{}^*(1-\lambda_1{}^{*2})\sin^2\frac{p_1}{2}\Big]. \qquad (A.21)$$

## APPENDIX B

We consider the correlator

$$\langle K(R)\rangle=\Big\langle\prod_{x=0}^{R-\hat{1}}\Big(\frac{1+\sigma_x\sigma_{x+1}}{2}\Big)\Big\rangle. \qquad (B.1)$$

This expression corresponds to a partition function with Hamiltonian (A.2), in which the horizontal bonds on the segment $[0,R]$ are infinite-the spins on this segments point in only one direction. Accordingly, in the dual representation (A.16), the bonds $\lambda_2^*$ that intersect the segment $[0,R]$ are equal to zero. Thus, the correlator (B.1) can be written in the form (A.5), in which the bonds $\lambda_{x\alpha}$, which intersect the segment $[0,R]$, are equal to zero. Therefore

$$\langle K(R)\rangle=\Big\langle\exp\Big\{-\lambda_2{}^*\sum_{x=0}^{R-\hat{1}}\bar{\psi}^{\alpha}_{x+\hat{2}}P_2^{\alpha\beta}\psi_x{}^{\beta}\Big\}\Big\rangle. \qquad (B.2)$$

This expression coincides, apart from the substitution $(-\lambda_2^*)\to(-2\lambda_2^*)$ in the argument of the exponential, with the expression for the correlator $\langle\sigma_0\sigma_R\rangle$, a detailed calculation of which is given in Ref. 17. The result is of the form

$$\langle K(R)\rangle\sim R^{-\zeta}\exp\{-R/r_c(n)\}, \qquad (B.3)$$

where

$$\zeta=-\int_{-\infty}^{+\infty}\frac{dt}{2\pi}\ln\Big(1-\frac{1}{2\,\mathrm{ch}^2\pi t}\Big)=\frac{3}{16},$$

and

$$r_c{}^{-1}(n)=-\frac{1}{2}\int_{-\pi}^{\pi}\frac{dp_1}{2\pi}\ln\{\det[1+\hat{g}(p_1)]\}, \qquad (B.4)$$

where the $2\times 2$ matrix $\hat{g}(p_1)$ is defined in terms of the matrix $\hat{G}(p)$ (A.11) (see Ref. 17):

$$g^{22}(p_1)=g^{44}(p_1)=\int_{-\pi}^{\pi}\frac{dp_2}{2\pi}G^{22}(p_1,p_2),$$

$$g^{24}(p_1)=\int_{-\pi}^{\pi}\frac{dp_2}{2\pi}G^{24}(p_1,p_2)e^{ip_2}, \qquad (B.5)$$

$$g^{42}(p_1)=\int_{-\pi}^{\pi}\frac{dp_2}{2\pi}G^{42}(p_1,p_2)e^{-ip_2}.$$

Using the definition (A.11), (A.12) as well as Eq. (A.19) it is easy to verify that, in first order in $n$,

$$r_c^{-1}(n)\approx -G^{*22}(\mathrm{x},\mathrm{x})=n, \qquad (B.6)$$

as it should be, since $n^{-1}$ is the mean distance between the solitons.

Somewhat more cumbersome is the calculation of the correlator $\langle K(R)\sigma(R)\rangle$, for which we have in place of (B.2) [we shall be interested henceforth only in power-law asymptotic forms, i.e., we shall assume that $R\ll n^{-1}$]

$$\langle K(R)\sigma(R)\rangle=\Big\langle\exp\Big\{-\lambda_2{}^*\sum_{x=0}^{R}\bar\psi^{\alpha}_{x+\hat 2}P_2^{\alpha\beta}\psi_x{}^{\beta}$$

$$-2\lambda_2{}^*\sum_{R}^{\infty}\bar\psi^{\alpha}_{x+\hat 2}P_2^{\alpha\beta}\psi_x{}^{\beta}\Big\}\Big\rangle. \qquad (B.7)$$

Following Ref. 17, we obtain from (B.7)

$$\langle K(R)\sigma(R)\rangle=\exp\Big\{-\sum_{n=1}^{\infty}n^{-1}\Pi_n\Big\}, \qquad (B.8)$$

where

$$\Pi_n=\sum_{x_1=1}^{r_c}\dots\sum_{x_n=1}^{r_c}\lambda(x_1)\dots\lambda(x_n)\,\mathrm{Sp}\{\hat G(\mathbf{x}_1-\mathbf{x}_2)\cdot\ldots\cdot\hat G(\mathbf{x}_n-\mathbf{x}_1)\} \qquad (B.9)$$

is a loop of order $n$, and

$$\lambda(x)=-1,\ 1<x<R,$$
$$\lambda(x)=-2,\ x>R. \qquad (B.10)$$

The Green functions in (B.8) are the Green functions (A.11) and (A.12) with zero mass, and the corresponding summation over $x$ is cut off at a correlation radius $r_c\sim m^{-1}$. Summing the diagonal (local) Green functions in (B.8) we obtain loops of the off-diagonal Green functions $G^{24}$ and $G^{42}$, and in place of (B.9) we have a function equal to $(-2)$ on the segment $[0, R]$ and to $(-2A)$ (see Eq. (3.12) in Ref. 17) at $x>r$. We can then verify that there are four contributions to the correlator $\langle K(R)\sigma(R)\rangle$.

The first contribution comes from the integration in the loops near the left end of the segment $[0, R]$ and yields $R^{-\zeta/2}$, just as in $\langle K(R)\rangle$. The second contribution stems from the integration in the loops over the segment $[R, R_c)$ near the left end, and yields $R_c^{-1/8}\sim\tau^{1/8}$. One more contribution comes from integration near the right end of the segment $[0, R]$, and is equal to $R^{-\zeta/2}$. Finally, the last contribution comes from the logarithmic integration near the right end of the segment $[0, R]$, in the loops in which some of the points are on the segment $[0, R]$ and some on the segment $[R, R_c]$. Summing in the loops the contributions from integrals of the form

$$(-2A)^l\int_R^{R_c}dx_1\dots dx_l\,G^{24}(x-x_1)G^{42}(x_1-x_2)\cdot\ldots\cdot G^{42}(x_l-x'), \qquad (B.11)$$

where the points $x$ and $x'$ lie on the segment $[0, R]$, we obtain the function

$$(-2)[(2\pi)^2(x-x')]^{-1}\ln\left|\frac{R-x}{R-x'}\right|.$$

Accordingly, the loops made up of these functions,

$$(-2)^{2k}\int_0^{R}dx_1\dots dx_n\left[\ln\left|\frac{R-x_1}{R-x_2}\right|\dots\ln\left|\frac{R-x_k}{R-x_1}\right|\right]$$

$$\times[(x_1-x_2)\dots(x_k-x_1)]^{-1}, \qquad (B.12)$$

make a contribution $R^{1/8}$. It is easy to verify that there are no other logarithmically diverging loops. We thus obtain

$$\langle K(R)\sigma(R)\rangle\sim R^{-\zeta+1/8}|\tau|^{1/8}. \qquad (B.13)$$

## APPENDIX C

A method for calculating the transition-temperature shift in the Ising model with impurity bonds was developed in Ref. 12. Our case is made complicated by the condition (A.17) or (A.19), which fixes the number of excited bonds on the chain, and this number must now be averaged over the configurations of the impurity bonds:

$$\overline{G^{*22}(x,x)}=-n. \qquad (C.1)$$

In addition, the horizontal and vertical bonds $J_\parallel$ and $J_\perp$ fluctuate differently. Calculation of the shift of the transition temperature reduces to calculation of the mass shift in the Green function $\overline{G(p_1,p_2)}$ averaged over the impurities.

We consider first the case when only the bond $J_\parallel$ fluctuates. Consider (C.1) can then be written in the form (see Ref. 12)

$$\int_{-\pi}^{\pi}\frac{d^2p}{(2\pi)^2}[1-\hat\Omega-\hat\Lambda(p_1,p_2)]^{-1}\hat\Lambda(p_1,p_2)=-n, \qquad (C.2)$$

where

$$\hat\Omega=\begin{vmatrix}0&0&0&0\\0&\Omega_2&0&0\\0&0&0&0\\0&0&0&\Omega_2\end{vmatrix}, \qquad (C.3)$$

$$\Omega_2=-\nu\frac{a^{*2}[-G^{*22}(0)]}{1+a^*[-G^{*22}(0)]}\approx\nu n a^{*2}, \qquad (C.4)$$

$$a^*=\frac{\bar\lambda_2{}^*-\lambda_2{}^*}{\lambda_2{}^*}=\exp\Big\{2\frac{J_\parallel-\mathcal{J}_\parallel}{T^{(0)}}\Big\}-1,$$
$$\bar\lambda_2{}^*=\exp\{-2\beta_c^{(0)}(\mathcal{J}_\parallel-\mu)\}. \qquad (C.5)$$

We now obtain in place of (C.1)

$$\int\frac{d^2p}{(2\pi)^2}\overline{G^{*22}(p_1,p_2)}-1-\Omega_2=-n, \qquad (C.6)$$

$$\hat G^*(\mathbf{p})=[1-\hat\Omega-\hat\Lambda(\mathbf{p})]^{-1}. \qquad (C.7)$$

Using (A.12) and (C.3) we obtain after some calculations

$$G^{*22}(p_1p_2)=\Big\{i\bar{\lambda}_2^*(1-\lambda_1^{*2})\sin p_2+\tilde{m}(1-\lambda_1^*)$$
$$+2\bar{\lambda}_2^*(1-\lambda_1^{*2})\sin^2\frac{p_2}{2}$$
$$+4\lambda_1^*(1-\Omega_2)\sin^2\frac{p_1}{2}\Big\}\Big\{4\lambda_1^*[(1-\Omega_2)^2-(\bar{\lambda}_2^*)^2]$$
$$\times\sin^2\frac{p_1}{2}+4\bar{\lambda}_2^*(1-\lambda_1^{*2})\sin^2\frac{p_2}{2}+\tilde{m}^2\Big\}^{-1}, \qquad \text{(C.8)}$$

$$\tilde{m}=1-\Omega_2-\bar{\lambda}_2^*-\lambda_1^*(1-\Omega_2)-\lambda_1^*\bar{\lambda}_2^*, \qquad \text{(C.9)}$$

$$\overline{\lambda_2^*}=\lambda_2^*+\nu(\tilde{\lambda}_2^*-\lambda_2^*)\equiv\lambda_2^*(1+\nu a^*). \qquad \text{(C.10)}$$

From the condition $\tilde{m}=0$ it follows that

$$\overline{\lambda_2^*}=(1-\Omega_2)(1-\lambda_1^*)(1+\lambda_1^*)^{-1}. \qquad \text{(C.11)}$$

Substituting (C.11) in (C.8) and then (C.8) in (C.6), we obtain after integration

$$\frac{1}{1-\Omega_2}\left[\frac{1+\lambda_1^{*2}}{2\pi\lambda_1^*}\arccos\left(\frac{2\lambda_1^*}{1+\lambda_1^*}\right)-\frac{(1+\lambda_1^*)^2}{4\lambda_1^*}+1\right]=n. \qquad \text{(C.12)}$$

From this we get

$$\lambda_1^*\approx\lambda_1^{*(0)}+\pi n\Omega_2, \qquad \text{(C.13)}$$

or

$$\frac{J_\perp}{T_c(\nu)}\simeq\frac{J_\perp}{T_c^{(0)}}+\frac{\pi}{2}\nu n^2\left(\exp\left\{2\frac{J_\parallel-\mathcal{J}_\parallel}{T_c^{(0)}}\right\}-1\right)^2, \qquad \text{(C.14)}$$

where $T_c^{(0)}$ is the transition temperature of the model without impurities. Owing the condition (C.1), there is no correction $\sim\nu n$ here. In the presence of fluctuations of $J_\perp$, however, this correction appears, simply because the transition temperature is defined in terms of the quantity

$$\bar{\lambda}_1^*=\lambda_1^*\left(1-\nu\frac{\bar{\lambda}_1^*-\lambda_1^*}{\lambda_1^*}\right)\approx\lambda_1^*\left[1+\pi n\nu\left(1-\frac{\mathcal{J}_\perp}{J_\perp}\right)\right]. \qquad \text{(C.15)}$$

It is easy to verify that as a result of the fluctuations of $J_\perp$ the main increment to $J_\perp/T_c$ is of the form

$${}^1/_2\pi\nu n(1-\mathcal{J}_\perp/J_\perp). \qquad \text{(C.16)}$$

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