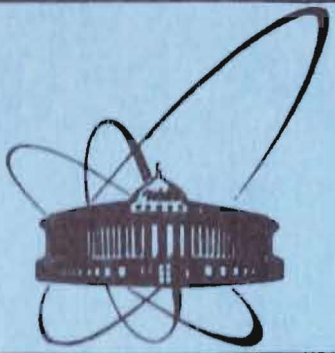

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THE EFFECTS DUE TO FINITE TEMPERATURE AND CHEMICAL POTENTIAL IN TWO-DIMENSIONAL FIELD THEORY MODELS AND POLYACETYLENE

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1. Introduction

The simplest linear conjugated polymer, trans-polyacetylene $(CH)_x$, can be treated as the one-dimensional Peierls-dimerized system with the half-filled band [1,2]. The spontaneous symmetry breaking (SSB) leads to the dimerized chains for any nonzero electron-phonon coupling strength. As a consequence of the ground-state twofold degeneracy, there exist topological solitons that can explain the physical properties of the trans-$(CH)_x$ [1].

The SSB exists in the main relativistic quantum field theory (RQFT) models. The investigation of the (1+1)-dimensional models with SSB has a specific interest. In the Gross-Neveu (GN) model the dynamical breaking of the discrete γ_5 symmetry occurs, whereas in the model φ^4 with fermions (φ_F^4) the reflection symmetry is spontaneously broken. The fermions in the GN and φ_F^4 models acquire the mass due to the interaction with the broken symmetry Bose field. The mass gap in the fermionic spectrum and the dimerization gap in the trans-$(CH)_x$ are equivalent.

In ref. [5] the SSB restoration in the RQFT models at finite temperature is considered. The growth of the fermion density and external fields leads to an analogous effects (see, for example, [6]). The corresponding analysis within the GN model has been performed in refs. [7,8]. If the symmetry restoration takes place, topological solitons disappear.

The influence of the finite temperature and electric field on the Peierls transition in the continuum Peierls model at $\rho = 1$, where ρ denotes the number of electrons on the elementary cell, is considered in ref. [9]. At zero temperature and $\rho \simeq 1$ the exact solution of the Peierls model in the self-consistent field approximation has been found in ref. [10]. The ground state includes the incommensurate solitonic lattice. The generalization to the finite temperatures is developed in refs. [11].

In our paper the SSB in the GN and φ_F^4 models at finite temperature T and fermion density n is investigated. The RQFT technique modified to finite T and n is used [12,13]. All calculations have been performed in the mean field approximation. We determine the critical values T_c and n_c above which the SSB are absent. In refs. [14,25] the analogy between continuum trans-$(CH)_x$ model and (1+1)-dimensional RQFT models has been developed. We show that this fortunate convergence takes place in the case of finite T and n. The effective potential in the GN model and the grand potential in the trans-$(CH)_x$ are equivalent. On this basis the new interpretation of the dielectric-metal transition in trans-$(CH)_x$ is presented. The φ^4 model (without fermions) is intensively used in the theory of structural phase transitions in the condensed matter physics. It is shown that the introduction of the fermionic terms in the Hamiltonian of the system gives rise to the soft phonon mode appearance at finite n.

2. The Gross-Neveu model

The Lagrangian of the model has the form [3]

$$\mathcal{L} = \sum_{p=1}^{N} \left[i \bar{\psi}^p \partial\!\!\!/ \psi^p \right] + \frac{g_{GN}^2}{2} \left(\sum_{p=1}^{N} \bar{\psi}^p \psi^p \right)^2 . \qquad (1)$$

The model contains N fermions with quartic interaction. ψ is a two-component spinor, $\bar{\psi} = \psi^+ \gamma_0$, $\partial\!\!\!/ = \partial_\mu \gamma^\mu$, $\mu = 0,1$, $\gamma_0 = \sigma_3$, $\gamma_1 = i\sigma_1$, σ_i are the Pauli matrices, g_{GN} is the dimensionless coupling constant. The Lagrangian (1) is invariant under the discrete chiral transformation $\psi \to \psi' = \gamma_5 \psi$ with $\gamma_5 = \gamma_0 \gamma_1$. It was found [3] that $\bar{\psi}\psi$ develops a nonvanishing vacuum expectation value at any nonzero coupling constant g_{GN}. Following [1], we can replace (1) by

$$\mathcal{L} = \sum_{p=1}^{N} \left[i \bar{\psi}^p \partial\!\!\!/ \psi^p - g_{GN} \sigma \bar{\psi}^p \psi^p \right] - \frac{1}{2} \sigma^2 , \qquad (2)$$

where a neutral scalar field σ is introduced. The equations of motion are

$$\left[i \partial\!\!\!/ - g_{GN} \sigma(x,t) \right] \psi^p(x,t) = 0 \qquad (3)$$

and

$$\sigma(x,t) = - g_{GN} \sum_{p=1}^{N} \bar{\psi}^p(x,t) \psi^p(x,t) . \qquad (4)$$

At $\sigma_0 \neq 0$, where $\sigma_0 = \langle 0 | \bar{\psi}\psi | 0 \rangle \neq \sigma_0(x)$ is a vacuum expectation value of the composed scalar field, the γ_5 invariance of (2) is broken. The interaction with the composed field σ leads to a mass gap $m_\psi = g_{GN} \sigma_0$ in the fermionic spectrum. The equations (3-4) admit in the statical case the kink solution [15].

$$\sigma(x) = \sigma_0 \tanh m_\psi x \qquad (5)$$

At finite temperature and chemical potential α the symmetry breaking parameter in the system is given by the T and α dependent quantity $\sigma_0(T,\alpha) = \langle\sigma\rangle$, where $\langle \dots \rangle$ denotes the grand canonical Gibbs ensemble averaging, rather than by the vacuum expectation value. Non-vanishing values of α lead to finite fermion or antifermion densities. This situation is naturally realized in condensed matter physics. The examples doped with donors or acceptors have the excess electrons (holes) and $\alpha \neq 0$.

To analyse the ground state we shall construct the effective potential of the system. Using the one-loop and mean field approximations we summarize all one-loop graphs (see Fig. 1) and obtain

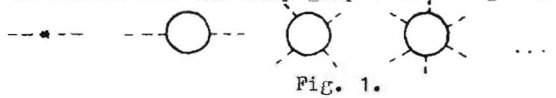

Fig. 1.

$$P_{eff}(\sigma) = \frac{1}{2}\sigma^2 - iN\sum_{n=1}^{\infty}\int\frac{d^2k}{(2\pi)^2}\frac{1}{n}\left(\frac{\lambda\sigma^2}{Nk^2}\right)^n , \qquad (6)$$

where the dimensionless parameter $\lambda = N g_{eff}^2$ is introduced. At finite T and α we must replace

$$k_0 \to i\omega_n , \quad \int\frac{dk_0}{2\pi} \to iT\sum_{n=-\infty}^{\infty} , \quad \text{where} \quad \omega_n = (2n+1)\pi T - i\alpha . \qquad (7)$$

Eq. (6) reduces to

$$P_{eff}(\sigma,T,\alpha) = \frac{1}{2}\sigma^2 - 2NT\int_0^{\infty}\frac{dk}{2\pi}\sum_{n=-\infty}^{\infty}\ln\frac{k^2+\omega_n^2+\frac{\lambda}{N}\sigma^2}{k^2+\omega_n^2} , \qquad (8)$$

The sum in (8) can be easily found

$$\sum_{n=-\infty}^{\infty}\ln(\omega_n^2+a^2) = -\frac{a}{T} + \ln\left[1+\exp\left(\frac{a-a}{T}\right)\right]\left[1+\exp\left(\frac{a+a}{T}\right)\right] . \qquad (9)$$

and we rewrite (8) in the form

$$P_{eff}(\sigma,T,\alpha) = \frac{1}{2}\sigma^2 - 2NT\int_0^{\infty}\frac{dk}{2\pi}\ln\frac{\left[1+\exp\left(\frac{\alpha-\varepsilon}{T}\right)\right]\left[1+\exp\left(\frac{\alpha+\varepsilon}{T}\right)\right]}{\left[1+\exp\left(\frac{\alpha-k}{T}\right)\right]\left[1+\exp\left(\frac{\alpha+k}{T}\right)\right]} , \qquad (10)$$

where $\varepsilon(k) = \sqrt{k^2+\frac{\lambda}{N}\sigma^2} = \sqrt{k^2+m_\psi^2}$.

The basic state of the system can be determined by examining the minimum of (10). Consequently, we must solve the equation

$$\frac{\partial P_{eff}}{\partial\sigma} = \sigma\left[1 - \frac{\lambda}{\pi}\int_c^{\infty}\frac{dk}{\varepsilon}\frac{\operatorname{sh}\frac{\varepsilon}{T}}{\left(\operatorname{ch}\frac{\varepsilon}{T}+\operatorname{ch}\frac{\alpha}{T}\right)}\right] = 0 . \qquad (11)$$

At $T=\alpha=0$ the ground state is twofold degenerate with the vacuum expectation value $g_{eff}\sigma = g_{eff}\sigma_0 = 2\Lambda\exp(-\pi/\lambda)$, where Λ is a cut-off momentum in (11). Hence at $\lambda \neq 0$ fermions have mass $m_\psi(0) = g_{eff}\sigma_0$. When the temperature is increased $m_\psi(T)$ decreases and tends to a zero value at $T \to T_c = \frac{\gamma m_\psi(0)}{\pi}$, where $\ln\gamma = \gamma_E$ is Euler's constant. At $T > T_c$ we have $\sigma \equiv 0$. The discrete γ_5 symmetry of (1) is restored. In this case the topological solitons (5) are absent.

Let us examine the case $\alpha \neq 0$. According to [8] we use the limit $T \to 0$. Then, we can rewrite (10) in the form

$$P_{eff}(\sigma,0,\alpha) = \frac{1}{2}\sigma^2 - \frac{N}{\pi}\left[\int_0^{\sqrt{\alpha^2-(g_{eff}\sigma)^2}} dk\,(\alpha-\varepsilon) + \int_0^{\infty} dk\,(\varepsilon-k) - \frac{\alpha^2}{2}\right] . \qquad (12)$$

It will be noted that at $\alpha < g_{eff}\sigma$ the first integral in (12) is absent. It is convenient to consider (12) in two cases.

1. Let us $\alpha < g_{eff}\sigma$. From (10) we have

$$P_{eff}(\alpha<g_{eff}\sigma) = \frac{1}{2}\sigma^2 + \frac{N}{2\pi}\left[\alpha^2 - \frac{(g_{eff}\sigma)^2}{2} - (g_{eff}\sigma)^2\ln\frac{2\Lambda}{g_{eff}\sigma}\right] . \qquad (13)$$

The extremum of (13) takes place when

$$\sigma\left[1 - \frac{\lambda}{\pi}\ln\frac{2\Lambda}{g_{eff}\sigma}\right] = 0 . \qquad (14)$$

From (14) we obtain two solutions: $\sigma = 0$ and $\sigma = \sigma_0 = m_\psi(0)/g_{eff}$.

2. Let us $\alpha > g_{eff}\sigma$. Then

$$P_{eff}(\alpha>g_{eff}\sigma) = \frac{N}{\pi}\left[\frac{\alpha^2}{2} - \frac{\alpha}{2}\sqrt{\alpha^2-(g_{eff}\sigma)^2} - \frac{(g_{eff}\sigma)^2}{4} + \frac{(g_{eff}\sigma)^2}{2}\ln\frac{\alpha+\sqrt{\alpha^2-(g_{eff}\sigma)^2}}{g_{eff}\sigma}\right] . \qquad (15)$$

The extremum points of (15) are $\sigma = 0$ and

$$\sigma^* = \sigma_0\sqrt{\frac{2\alpha}{g_{eff}\sigma} - 1} , \qquad (16)$$

where $\alpha > m_\psi(0)/2$. Summarizing all the solutions we have the qualitative picture given in Fig. 2 (see below). The effective potential at the extremum points has the forms:

$$P_{eff}(0,\alpha) = 0\,,$$
$$P_{eff}(\sigma_0,\alpha) = \frac{N}{\pi}\left[\frac{\alpha^2}{\lambda} - \frac{(g_{cm}\sigma_0)^2}{4}\right], \qquad (17)$$
$$P_{eff}(\sigma,\alpha) = \frac{N}{\pi}(\alpha - g_{cm}\sigma_0)^2\,.$$

In accordance with (17) at $\alpha < \alpha_c$, where $\alpha_c = m_\varphi(0)/\sqrt{2}$ the minimum of P_{eff} takes place at the point $\sigma = \sigma_0$ whereas at $\alpha \geq \alpha_c$ $\sigma = 0$. There is first order phase transition [18,26].

In ref. [8] the critical density corresponding to the point A in Fig. 2 was obtained. It is clear that the result [8] is incorrect. At $\alpha \geq \alpha_c$ the topological solitons disappear. On the other hand at $T = 0$ and $\alpha < \alpha_c$ the width and the amplitude of solitons are α-independent. Using the connection between fermion density and chemical potential $n = \frac{2}{\pi}\int_0^\infty dk\left[\exp\left(\frac{\varepsilon-\alpha}{T}\right)+1\right]^{-1}$ we have in the critical region at $T \to 0$ $n_1 = N\alpha/\pi$. Hence

$$n_c = \frac{N m_\varphi(0)}{\sqrt{2}\,\pi} \qquad (18)$$

3. The φ^4 model with fermions

The Lagrangian has the form

$$\mathcal{L} = \frac{1}{2}(\partial_\nu\varphi)^2 + \frac{1}{2}\mu_0^2\varphi^2 - \frac{\lambda}{4}\varphi^4 + \sum_{\rho=1}^{N}\bar\psi^\rho(i\partial\!\!\!/ - g\varphi)\psi^\rho\,. \qquad (19)$$

Contrary to (1) the model (19) contains scalar bosons as the fundamental fields. We pay attention to the dynamical term for the scalar field φ in (19). In what follows we shall consider only the case N=2.

It is clear that even at the classical level the potential energy of (19) has minimum at $\sigma_0 = \langle 0|\varphi|0\rangle = \pm\mu_0/\sqrt{\lambda}$. The Lagrangian (19) is invariant under the discrete chiral transformation $\psi \to \gamma_5\psi$ and $\varphi \to -\varphi$. In the ground state the reflection symmetry is distorted. After the shift $\varphi = \varphi' + \sigma_0$ the field φ' has a usual vacuum expectation value $\langle 0|\varphi'|0\rangle = 0$. The twofold degeneracy of the ground state leads to topological solitons

$$\varphi(x) = \sigma_0 \tanh\frac{\mu_0 x}{\sqrt{2}}\,. \qquad (20)$$

We construct now the effective potential of the system with Lagrangian (19). The quantum corrections due to fermionic as well as bosonic loops should be taken into account. The method developed in ref. [12] for four-dimensional models is used. In the two-dimensional case

only logarithmic divergences from the one-loop graphs persist. In order to justify the use of perturbation theory it will be assumed that $\lambda, g^2 \ll \mu_0^2$. In this case we shall consider only the one-loop graphs. Following [12] at finite temperature and chemical potential we have

$$P_{eff}(\varphi) = P(\varphi) + \frac{1}{2}C(T,\alpha)\varphi^2, \qquad (21)$$

where $P(\varphi) = -\frac{\mu_0^2}{2}\varphi^2 + \frac{\lambda}{4}\varphi^4$, $C(T,\alpha) = 3\lambda I_B(T,\alpha) - 2g^2 I_F(T,\alpha)$

and

$$I_B(T,\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{2\omega_B}\coth\frac{\omega_B}{2T}\,, \qquad I_F(T,\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{\omega_F}\,\frac{\sinh\frac{\omega_F}{T}}{\left(\cosh\frac{\omega_F}{T} + \cosh\frac{\alpha}{T}\right)},$$

$$\omega_B = \sqrt{k^2 + m_\varphi^2(T,\alpha)}\,, \qquad \omega_F = \sqrt{k^2 + m_\varphi^2(T,\alpha)}\,.$$

$C(T,\alpha)$ is divergent logarithmically at $k \to \infty$. After renormalization one can obtain

$$P_{eff}(\varphi) = P_{ren}(\varphi) + \frac{1}{2}C^R(T,\alpha)\varphi^2\,, \qquad (22)$$

where

$$C^R(T,\alpha) = 3\lambda I_B^R(T,\alpha) - 2g^2 I_F^R(T,\alpha) \qquad (23)$$

and

$$I_B^R(T,\alpha) = I_B(T,\alpha) - I_B(0) = \frac{1}{2\pi}\ln\frac{m_\varphi(0)}{m_\varphi(T,\alpha)} + \frac{1}{\pi}\int_0^\infty\frac{dk}{\omega_B}\left(e^{\frac{\omega_B}{T}}-1\right)^{-1}, \qquad (23')$$

$$I_F^R(T,\alpha) = I_F(T,\alpha) - I_F(0) = \frac{1}{2\pi}\ln\frac{m_\varphi(0)}{m_\varphi(T,\alpha)} - \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{\omega_F}F\left(\frac{\omega_F}{T},\frac{\alpha}{T}\right), \qquad (23'')$$

$$F\left(\frac{\omega_F}{T},\frac{\alpha}{T}\right) = \frac{1}{\left[\exp\left(\frac{\omega_F-\alpha}{T}\right)+1\right]} + \frac{1}{\left[\exp\left(\frac{\omega_F+\alpha}{T}\right)+1\right]}\,.$$

$P_{ren}(\varphi)$ is just the original polynomial $P(\varphi)$ but with masses replaced by renormalized values at $T = \alpha = 0$, i.e., $\mu_0^2 \to \mu^2 = \mu_0^2 + 3\lambda I_B(0) - 2g^2 I_F(0)$. The extremum of (22) takes place in the case

$$\left.\frac{\partial P_{eff}}{\partial\varphi}\right|_{\varphi=\sigma} = \sigma\left[\lambda\sigma^2 - \mu^2 - Q^R(T,\alpha|\sigma)\right] = 0\,. \qquad (24)$$

Note that the mass of the Bose field has the form

$$m_\varphi^2(T,\alpha) = \frac{\partial^2 P_{eff}}{\partial\varphi^2}\Big|_{\varphi=\sigma} = -\mu^2 + 3\lambda\sigma^2 + Q^R(T,\alpha|\sigma) \quad . \qquad (25)$$

The fermionic mass $m_\psi(T,\alpha) = g\sigma(T,\alpha)$.

At $T=\alpha=0$ we have $m_\varphi^2(0) = 3\lambda\sigma^2(0) - \mu^2 = 2\mu^2$, where $\sigma(0) = \pm\mu/\sqrt{\lambda}$ is a renormalized value of the vacuum expectation. For the trivial solution of (24) $\sigma = 0$ we obtain $m_\psi = 0$ and $m_\varphi^2(T,\alpha) = -\mu^2 + Q^R(T,\alpha|0)$. At $T=\alpha=0$ the value of $Q^R(0)$ vanishes. Hence Bose field φ has a nonphysical mass and SSB takes place.

Consider now the nontrivial solutions of (24). It is convenient to rewrite (24) in the form

$$m_\varphi^2(T,\alpha) - 2\mu^2 + 2G^R(T,\alpha|\sigma) = 0. \qquad (26)$$

We examine first the case $\alpha = 0$. In the approximation $T \gg m_\varphi(T,\alpha)$, $m_\psi(T,\alpha)$ the integrals in (24) have the form /13/

$$I_B^R(T) = \frac{1}{2\pi}\ln\frac{m_\varphi(0)}{4\pi T} + \frac{T}{2m_\varphi(T)} + \frac{1}{2\pi}\gamma_E + O\left[\left(\frac{m_\varphi(T)}{T}\right)^2\right],$$

$$I_F^R(T) = \frac{1}{2\pi}\ln\frac{m_\psi(0)}{\pi T} + \frac{1}{2\pi}\gamma_E + O\left[\left(\frac{m_\psi(T)}{T}\right)^2\right].$$

Thus, we obtain the equation

$$m_\varphi^3(T) - pm_\varphi(T) + q = 0, \qquad (27)$$

where $p = 2\mu^2 - \frac{3\lambda}{\pi}\ln\frac{m_\varphi(0)}{4\pi T} - \frac{3\lambda}{\pi}\gamma_E + \frac{2g^2}{4\pi}\ln\frac{m_\psi(0)}{\pi T} + \frac{2g^2}{\pi}\gamma_E$, $q = 3\lambda T$. At $D \le 0$ where $D = \left(\frac{p}{3}\right)^3 + \left(\frac{q}{2}\right)^2$ there is at least one positive root of (27). The critical temperature obtained from the provision $D = 0$ has the form

$$T_c = \frac{4\sqrt{2}\,\mu^3}{9\sqrt{3}\lambda}\left[1 - \frac{3}{2}B(T=T_c)\right], \qquad (28)$$

where

$$B(T=T_c) = \frac{3\lambda}{2\pi\mu^2}\left[\ln\frac{9\sqrt{3}\lambda}{16\pi\mu^2} + \gamma_E\right] - \frac{g^2}{\pi\mu^2}\left[\ln\frac{9\sqrt{3}\lambda\, m_\psi(0)}{4\sqrt{2}\pi\mu^3} + \gamma_E\right]$$

is a small correction to $T = T_c$. It will be noted that at $\alpha = 0$ the contribution from the boson loops is crucial. At $g = 0$ the result (28) is consistent with that of refs./16/. At the critical point the order parameter σ has a jump from $\sigma(T\to T_c^-) = 0{,}57\,\sigma(0)$ to $\sigma = 0$ at $T \ge T_c$. Analogously, $m_\psi(T\to T_c^-) = 0.57\, m_\psi(0)$ whereas $m_\psi(T>T_c) = 0$. The mass of the Bose field can be obtained from

(27). We have $m_\varphi(T\to T_c^-) = \left(\frac{3\lambda T_c}{2}\right)^{1/3} \simeq 0{,}2\mu$ or $m_\varphi^2(T\to T_c^-) \simeq \frac{1}{3}m_\varphi^2(0)$. At $T > T_c$ the order parameter $\sigma = 0$ and $m_\varphi^2(T>T_c) \simeq -\mu^2 + (3\lambda T/2\, m_\varphi(T))$ i.e., $m_\varphi^2(T>T_c) \simeq 0{,}1\, m_\varphi^2(0)$. Thus, the mass of the field φ has a jump at $T = T_c$ and tends to a nonzero value. This result is consistent with the assumption that at the structural phase transition in a one-dimensional system with the Hamiltonian φ^4 soft phonon mode is absent. Note that in this case in (19) φ is a phonon field.

Consider (24) at $\alpha \neq 0$. At $T \to 0$ we have $I_F^R(0,\alpha) = \frac{1}{2\pi}\ln\frac{m_\psi(0)}{2\alpha}$ and $I_B^R(0,\alpha) \to 0$. Then Eq. (24) has the form $\lambda\sigma^2 = \mu^2 - \frac{g^2}{4}\ln\frac{2\alpha}{m_\psi(0)}$. Using the equality $\eta = 2\alpha/\pi$ we have

$$\eta_c = \frac{m_\psi(0)}{\pi}\exp\left(\pi\mu^2/g^2\right). \qquad (29)$$

As opposed to the GN model the model φ_F^4 has a new interesting limit. In the case $T \neq 0$ we obtain for $T \gg m_\psi(T,\alpha)$ in the critical region

$$I_F^R(T,\alpha) \simeq \frac{1}{2\pi}\left[\ln\frac{m_\psi(0)}{T} - \bar{\alpha}\right], \qquad (30)$$

where $\bar{\alpha} = \frac{\alpha}{T}$. Thus, using the leading terms in (23) we have

$$Q^R(T,\alpha) = \frac{3\lambda T}{2\, m_\varphi(T,\alpha)} + \frac{g^2}{4}\bar{\alpha}. \qquad (31)$$

Eq. (26) takes the form

$$m_\varphi^3(T,\alpha) - \left(2\mu^2 - g^2\frac{\eta}{T}\right)m_\varphi(T,\alpha) + 3\lambda T = 0. \qquad (32)$$

From (32) one finds that

$$\eta_c = \frac{2\mu^2}{g^2}T_c - \frac{3\left(\frac{3\lambda}{2}\right)^{1/3}}{g^2}T_c^{5/3}. \qquad (33)$$

Note that the first and second terms in (33) are connected with the contributions from fermionic and bosonic loops respectively. At $\lambda \sim g^2 \ll \mu^2$ the first term in (33) is crucial and both $\sigma(T_c,\eta_c)$ and $m_\varphi(T_c,\eta_c)$ tend to a zero value /17/. If we return to the structural phase transition then this result implies the appearance of the soft phonon mode.

4. The polyacetylene model

The polyacetylene model /1/ may explain the electrical, magnetic, optical and transport properties of the $(CH)_x$ chains on the basis of the solitonic mechanism. The Hamiltonian of the model has the form

$$H = \frac{M}{2}\sum_n \dot{y}_n^2 + \frac{\varkappa}{2}\sum_n (y_{n+1} - y_n)^2 - \sum_{n,s} t_{n,n+1}\left(c^+_{n+1,s} c_{n,s} + h.c.\right), \quad (34)$$

where $c^+_{n,s}$ ($c_{n,s}$) creates (annihilates) a banding π electron of spin S at site n, y_n is a real, scalar, Bose field describing the coordinate displacement of the n-th (CH) group, $\varkappa$ is a spring constant, M is the total mass of the (CH) group. In the tight-binding approximation a hopping integral $t_{n,n+1}$ has the form $t_{n,n+1} = t_0 - \bar{\gamma}(y_{n+1} - y_n)$, where t_0 is the hopping integral for the undimerized chain and $\bar{\gamma}$ is the electron-phonon coupling constant. At $\bar{\gamma} = 0$ the Hamiltonian (34) is invariant under transformation $y_n \to -y_n$. At $\bar{\gamma} \neq 0$ the basis state is twofold degenerate. That is consistent with the Peierls theorem for the quasi-one-dimensional systems. The electronic spectrum exhibits the energetical gap ($2\Delta_0 \simeq 1.4$-1.8 eV) and $(CH)_x$ is a dielectric. The change of the lattice period gives rise to a charge density wave (CDW) with the wave vector $k = 2k_F = \pi/a_0$ where a_0 is a lattice constant. According to [1] the deviations in a pure bond alternated conformations lead to topological solitons. In the continuum polyacetylene model the soliton solution has the form [2]

$$\Delta(x) = \Delta_0 \tanh\frac{\Delta_0 x}{v_F} \quad (35)$$

analogous to (5). In (35) $v_F = 2t_0 a_0$ the Fermi velocity, $\hbar = 1$.

Consider now the influence of the finite temperature and an electron density increase on the ground state of the system. In the mean field approximation the thermodynamic grand potential has the form

$$\Omega(\Delta, T, \alpha) = -\frac{2T}{N}\sum_{\ell=1,2}\sum_q \ln\left[1 + \exp\left(\frac{\alpha - \varepsilon_\ell}{T}\right)\right] + \frac{\Delta^2}{4\pi t_0 g^2}, \quad (36)$$

where $\varepsilon_{1,2} = \pm\sqrt{(\Delta\sin q)^2 + (2t_0\cos q)^2}$, $a_0 = 1$, $q = \frac{2\pi n}{N}$ ($n = 0, \pm 1, \ldots \pm\frac{N}{4}$), Δ is a gap in the electronic spectrum, N is a number of atoms in the chain, $g^2 = \frac{2\bar{\gamma}^2}{\pi\varkappa t_0}$, α is the chemical potential. The uniform dimerization is considered $\Delta \neq \Delta(x)$. In the continuum limit we obtain from (36)

$$\Omega(\Delta, T, \alpha) = -\frac{2T}{\pi v_F}\int_0^{Kv_F} dq \ln\left[1 + \exp\left(\frac{\alpha - \varepsilon}{T}\right)\right]\left[1 + \exp\left(\frac{\alpha + \varepsilon}{T}\right)\right] + \frac{\Delta^2}{4\pi t_0 g^2}, \quad (37)$$

where the electronic spectrum $\varepsilon = \sqrt{q^2 + \Delta^2}$ is linearized in the vicinity of the Fermi points, K is a cutoff momentum. Note that the grand potential (37) is an analog of the effective potential (10). Thus the connection between continuum $(CH)_x$ and GN models takes place at finite T and α. Contrary to RQFT models the cutoff momentum in (37) has the natural sense due to the Fermi points. The full width of the Brillouin band is $W = 2\sqrt{K^2 v_F^2 + \Delta^2} \simeq 2Kv_F = 4t_0$. The extremum condition of (37) is

$$\frac{\partial\Omega(\Delta, T, \alpha)}{\partial\Delta} = \Delta\left(1 - 2g^2\int_0^{Kv_F}\frac{dq}{\varepsilon}\frac{\operatorname{sh}\frac{\varepsilon}{T}}{\left(\operatorname{ch}\frac{\varepsilon}{T} + \operatorname{ch}\frac{\alpha}{T}\right)}\right) = 0 \quad (38)$$

The parameters t_0 and g in the $(CH)_x$ model are well estimated. Eq. (38) was carried out numerically (see Figs. 2,3).

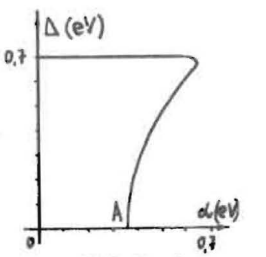

Fig. 2.

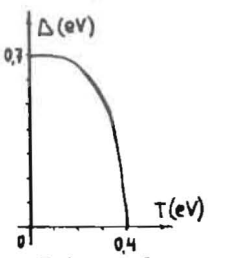

Fig. 3.

It will be noted that the conditions (38) and (11) are equivalent. Hence the analytical investigation of (38) is compared with that of (11). The results are the following. At $\alpha = 0$ the gap $\Delta(T)$ decreases from the value $\Delta(0) = 0.7$ eV to $\Delta = 0$ for $T = T_c = \frac{\gamma\Delta_0}{\pi}$ according to Fig. 3. At $\alpha \neq 0$ and $T \to 0$ ($\alpha \gg T$) the two limits take place. At $\Delta > \alpha$ the minimum of (37) occurs at $\Delta(0) = We^{\exp\left(-\frac{1}{2g^2}\right)} \simeq 0.7$ eV. At $\Delta < \alpha$ the extremum points are $\Delta = 0$ and $\Delta^* = \Delta(0)\sqrt{\frac{2\alpha}{\Delta(0)} - 1}$. These solutions are in complete agreement with the lines in Fig. 2. For the numerical investigation the interval $250K < T < 350K$ was used. All the results are as a matter of fact temperature independent.

At $\alpha > \alpha_c$, where $\alpha_c = \frac{\Delta_0}{\sqrt{2}}$, the symmetry of the system is restored. Using the connection $n = 2\alpha/\pi v_F$ we obtain the critical density

$$n_c = \frac{\sqrt{2}\,\Delta(0)}{\pi v_F}. \quad (39)$$

Note that if the value $T_c \simeq 4000K$ is remarkably higher comparing to

the fusion temperature of $(CH)_x$, then the critical density (39) is in good agreement with experimental data in doped trans-$(CH)_x$ chains. Let us $\gamma_c = n_c/n_0$ where $n_0 \sim 1/a_0$ is a density of π electrons in the pure undeformed $(CH)_x$. According to (39) the value γ_c interpolates between $0.063 < \gamma_c < 0.09$ at $0.7\ eV < \Delta(0) < 0.9\ eV$. As $\gamma > \gamma_c$ the gap in the electronic spectrum and amplitude solitons (35) disappear. In the limit $\Delta \to 0$ all π bounds are destroyed and the system transforms to a metal. We proposed in ref.[18] that all π electrons are electrical carriers in this case. Several experimental results have been explained quite convincingly within this proposal. In ref.[19] the electrical conductivity of trans-$(CH)_x$ with AsF_5 doping was measured. In the region $0.01 < \gamma < 0.07$ the conductivity increases from the value $\sigma = 10^{-5}(\Omega \cdot cm)^{-1}$ to $\sigma = 2.2\ 10^{2}(\Omega \cdot cm)^{-1}$. Above doping levels of $\gamma \simeq 0.07$ a metallic behaviour is observed.

The measurement of the paramagnetic Pauli susceptibility χ_p indicated that at $0.0005 < \gamma < 0.05$ the value χ_p vanishes whereas at $\gamma \to 0.07$ the Pauli contribution abruptly increases[20]. Above $\gamma = 0.07$ the value χ_p is in agreement with that for the metal with half-filled band. The increase in χ_p above $\gamma = 0.07$ was discussed as a consequence of closing the Peierls gap[20]. Similar results were obtained in both optical gap absorption[21] and thermopower[22] experiments.

However, it was shown in refs.[10,11] that at $\gamma < \gamma_c$ and $T = 300K$ the soliton lattice phase is realized as a basis state of the Peierls system. At $\gamma > \gamma_c$ there is a continuous transition to the incommensurate CDW. The gap in the electronic spectrum never closes, and no metal transition takes place.

Note that the integrable model considered in refs.[10,11] differs from the primary trans-$(CH)_x$ model[1]. In the continuum approximation the static equations of the model[1] contain the terms Δ_{xx}, ψ_{xx}, $\Delta_x \psi_x$, ... (see ref.[27]) which have been droped in refs.[10, 11]. At sufficiently high value of γ the role of these terms increases. The system becomes non-integrable and the proposal about a soliton lattice formation in the highly doped trans-$(CH)_x$ is opened to speculation. On the other hand in ref.[22] the metal transition in a one-dimensional trans-$(CH)_x$ chains has been obtained in accordance with the above-mentioned mechanism. The further increase of γ can lead to the incommensurate CDW phase transition.

Thus, we suppose that there is the small region of the doping

level when the doped trans-$(CH)_x$ examples have the metallic properties. The size of this region is connected with the doping process, type of the dopand, etc. (It seems that in the case of the Iodine dopands this region is absent). In the case of inhomogeneous distribution of the dopand the metallic islands with the critical value γ_c are formed. In the homogeneous case the first order phase transition takes place at $\gamma = \gamma_c$ and all π-bonds are destroyed.

The temperature Green function technique allows us to study the influence of quantum fluctuations of the Bose field on the structural phase transition. Following (28) the value $T_c = 0.385 E_K^0$ where $E_K^0 = \frac{2\sqrt{2}\mu}{3\lambda^2}$. The phenomenological model φ^4 was used to describe the polyacetylene properties[24]. Taking into account the value of $E_K^0 = \frac{4\Delta(0)}{3\pi}$ [24] we obtain the critical temperature $T_c^* = 0.16\,\Delta(0)$. In the GN model we had $T_c = \frac{\Delta(0)}{\pi} = 0.57\,\Delta(0)$.

Thus, $T_c^*/T_c = 0.28$. This result is in good agreement with the proposal that the critical temperature is decreased to a quarter of T_c upon including the Bose-fields fluctuations (see ref.[23]).

In conclusion we note that the fortunate convergence between condensed matter and relativistic field theories gives rise to the new principial results. We hope that this will stimulate new investigations in this area.

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Эффекты, обусловленные конечными значениями температуры и химического потенциала в некоторых двумерных полевых моделях и полиацетилене

В приближении среднего поля на основе формализма Мацубары с использованием диаграммной техники Фейнмана исследована структура основного состояния в континуальной модели транс-полиацетилена и двумерных /1+1/ моделях квантовой теории поля при конечных значениях температуры T и химического потенциала фермионов α. Получены критические значения T_c и α_c, при которых восстанавливается симметрия системы, спонтанно нарушенная при $T = \alpha = 0$. Показана возможность существования мягкой фононной моды в легированных одномерных проводниках, испытывающих структурный фазовый переход. Предложена новая интерпретация перехода диэлектрик-металл в полиацетилене.

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The Effects Due to Finite Temperature and Chemical Potential in Two-Dimensional Field Theory Models and Polyacetylene

In the mean field approximation using the diagrammatic Feynman technique, the structure of the ground state in both the continuum polyacetylene model and two-dimensional quantum field theory models at finite temperature T and chemical potential of fermions α is investigated. The critical values T_c and α_c are obtained. It is found that a symmetry which is broken at $T = \alpha = 0$ can be restored by raising T or α above critical values. The common features for the condensed matter and relativistic field theories are observed. It is shown that soft phonon mode in the one-dimensional model for structural phase transitions in the doped conductors can be presented. The new interpretation of the dielectric-metal transition in the doped trans-polyacetylene is introduced.

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

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