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THE DYNAMICAL EFFECTS IN THE GROSS-NEVEU AND POLYACETYLENE MODELS

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The physical characteristics of the moving solitons in the Gross-Neveu and polyacetylene models are calculated. It is found that the contributions to the charge and mass of solitons due to motion take place. In the case of the polaronic excitations the dynamic correction to the mass has a remarkable value (~37%). In the Gross-Neveu model the complete dynamical mass of solitons is only due to the fermion dynamics.

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

Динамические эффекты в моделях Гросса-Невье и полиацетилена

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Обсуждается модификация физических характеристик движущихся солитонов в моделях Гросса-Невье и полиацетилена. Вычислены поправки к заряду и массе солитонов, обусловленные их движением. В случае поляронного возбуждения динамическая поправка к массе весьма существенна /~37%/. В модели Гросса-Невье учет эффекта движения приводит к возникновению динамической массы солитонов.

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1. It was shown in refs.[1,2] that in the mean field approximation the static equations of motion in both the n=2 Gross-Neveu (GN) model field theory and the continuum trans-polyacetylene $(CH)_x$ model are equivalent. Some important corollaries of this connection have been investigated in refs.[1,3]. In ref.[4] the static solutions (kink, polaron) to the semiclassical equations of the GN model were constructed. The analogous static localized excitations are contained in $(CH)_x$ and play a remarkable role in describing the physical properties of trans - $(CH)_x$ chains. The dynamical properties of the GN and $(CH)_x$ models are quite different. The discrepancy is because of the distinct

physical background of the scalar field $\sigma(x,t)$ in the GN model and of the optical phonon field $\Delta(x,t)$ in $(CH)_x$. The σ field is an auxiliary composite object that does not describe the real bosons because the kinetic term σ_t^2 is absent in the GN model. The whole dynamics of the σ field is due to fermions (when the fermion quantum corrections are included), whereas in $(CH)_x$ the field $\Delta(x,t)$ has a kinetic term Δ_t^2.

As a consequence, the dynamical equations of motion for both models have a sufficiently different form. So, the complete system of equations of the GN model are invariant under the Lorentz transformations whereas it is not the case for the $(CH)_x$ model. It was shown in ref. [5] that in the limit of slowly moving solitons the dynamical properties of both models are formally equivalent, i.e., the system of equations of motion in $(CH)_x$ is reduced to that in the GN model and has the form

$$
\begin{aligned}
i u_t(x,t) &= -i V_F u_x(x,t) + \Delta(x,t) v(x,t) \\
i v_t(x,t) &= i V_F v_x(x,t) + \Delta(x,t) u(x,t)
\end{aligned}
\tag{1a}
$$

together with the self-consistent gap equation

$$
\Delta(x,t) = -(\lambda \pi V_F) \sum_{k,s}{}' (u_k^*(x,t) v_k(x,t) + v_k^*(x,t) u_k(x,t)). \tag{1b}
$$

Here, the electronic wave functions $u(x,t)$, $v(x,t)$ are normalized to unity $\int_{-\infty}^{\infty} dx(|u_k(x,t)|^2+|v_k(x,t)|^2)=1$. The summation in (1b) is over the two-spin states for every energy level up to the Fermi energy, that is chosen to be zero. In (1) V_F and λ are the Fermi velocity and the effective electron-phonon coupling constant, respectively. The transition to the GN model is obtained by making the transformations

$$
u \to \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2), \quad v \to \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2), \; \Delta \to g_{GN}\sigma, \quad \lambda\pi V_F \to g_{GN}^2, \quad V_F \to C,
$$

$s \to a$, where $\psi = \binom{\psi_1}{\psi_2}$ is a two-component Dirac spinor, g_{GN} and C are the coupling constant and light velocity, respectively; $a=\{1,..n\}$ is the internal SU(n) symmetry index.

As in the static case, there are three classes of solutions to eqs.(1). The first class corresponds to the homogeneous ground state $\Delta \equiv \Delta_0 = W\exp(-1/2\lambda)$. In $(CH)_x$ W is the full band width, $W=2k_F V_F$, where k_F is a Fermi momentum. In the GN model $W=2\Lambda$, where Λ is an unphysical cut-off introduced to make the theory finite. The electron wave functions in the valence band are the usual plane waves with density $\rho_k^o = \frac{1}{2\pi}$. The second class of solutions in $(CH)_x$ are the kinks. The explicit forms for the wave functions are given in ref.[5] . The third class of solutions are "polarons". The moving polaron can be obtained in an analogous manner using the invariance of eqs.(1) under the Lorentz transformation. The precise form of these solutions would be published in a separate article. Note that the kink solution has a zero energy bound state (E=0) in the fermion energy spectrum whereas the polaron solution has two symmetrical discrete levels at $E=\pm\omega_0$.

In our article the physical characteristics of the moving kink and polaron (the energy of formation, mass, charge) are calculated.

2. In the presence of an inhomogeneous deformation the change in the local electronic density can be written in the form

$$\Delta\rho(\xi) = \sum_{i=1}^{r} n_{B_i}\, \rho_{B_i}^{s}(\xi) + \sum_{k,\alpha} [\rho_k^{s}(\xi) - \rho_k^{o}(\xi)] , \qquad (2)$$

where the term $\rho_{B_i}^{s}(\xi)$ is due to the i-th bound state with the occupation number n_{B_i} , and $\rho_k^s(\xi)$ is the contribution of the negative energy scattering states. The electric charge of soliton is defined as $Q = e\int \Delta\rho(\xi)d\xi$. In the case of the moving kink, we obtain

$$Q = e(n_0 - \frac{n}{\pi}\,\mathrm{arctg}\,\frac{W\sqrt{1-\beta^2}}{2\Delta_0}), \qquad (3)$$

where $\beta = v_s/V_F$, v_s is a soliton velocity, n_0 is an occupation number of the discrete level at E=0. In the limit $W\to\infty$ we come to the result $Q_0 = e(n_0 - \frac{n}{2})$. In $(CH)_x$ $n=2$ and $Q_0 = e(n_0 - 1)$. When $n_0 = 1$, the solitonic charge is $Q_0 = 0$ whereas the spin $s = 1/2$. For $n = 1$ we have $Q_0 = \pm\frac{1}{2}|e|$, i.e., the effect of the fermion charge fractionalization in the presence of a soliton takes place. At finite value of W using the approximation $\delta \ll 1$,where $\delta = \frac{\Delta_0}{W}$, we obtain from eq.(3) that $Q = Q_0 + \delta Q$, where $\delta Q = e\frac{2n\Delta_0}{\pi W\sqrt{1-\beta^2}}$. Thus, even in the case of a neutral soliton a small charge proportional to δ appears in agreement with the result of paper [2]. In $(CH)_x$ we need to use the limit $\beta^2 \ll 1$. In this case the contribution to the charge of kink due to the velocity parameter β is additionally reduced by the small parameter δ . Note that for $(CH)_x$ $\delta \simeq 0.07$.

The kink creation energy can be calculated on the basis of the method developed in ref.[4]

We obtain

$$E_s = \frac{n\Delta_0}{\pi} + \frac{\Delta_0}{\pi\lambda}\frac{\beta^2}{\sqrt{1-\beta^2}}, \qquad (4)$$

where the first term corresponds to the well-known creation energy of the static kink[2,4]. The second term determines the dynamical correction to the mass of the kink excitation. At small values of β we have $\delta M_s = \frac{2\Delta_0}{\pi\lambda V_F^2}$. This important result implies that in the GN model, where the kinetic term is absent and as consequence $M_s = 0$, the finite dynamical mass of a kink appears. In $(CH)_x$ $M_s = \frac{M\Delta_0^3}{3\pi K\lambda V_F^2} \simeq 6\, m_e$, where M and K are the parameters of the $(CH)_x$ model and m_e is an electron mass. Thus, in $(CH)_x$ we have $\delta M_s \simeq 0.09 M_s$, i.e., the correction is considerable (~10%) contrary to the statement of the authors in ref.[6].

3. Let us propose that the polaronic level $E = -\omega_0(\omega_0)$ has the occupation number $n(n_0)$ respectively. The change in the local density in the presence of a polaronic deformation takes the form

$$\Delta\rho(\xi) = \frac{K_p}{4}(\mathrm{sech}^2 K_p\xi_+ + \mathrm{sech}^2 K_p\xi_-)\{(n_0+n) - \frac{2n}{\pi}\sqrt{1-\beta^2}\,\mathrm{arctg}\frac{W}{2K_0V_F} + \qquad (5)$$

$$+\beta^2\frac{2n}{\pi}\frac{K_0V_F^2}{[K_0^2V_F^2(1-\beta^2)-\Delta_0^2]}[\frac{\Delta_0}{K_0V_F}\mathrm{arctg}\frac{W\sqrt{1-\beta^2}}{2\Delta_0} - \sqrt{1-\beta^2}\,\mathrm{arctg}\frac{W}{2K_0V_F}]\},$$

where $\xi_\pm = x - v_p t + x_0$, v_p is a polaron velocity, $K_p = \frac{K_0}{\sqrt{1-\beta^2}}$ and $K_0V_F = \sqrt{\Delta_0^2-\omega_0^2}$, $\beta = v_p/V_F$. In the limit case $W \to \infty$, we obtain from eq. (5) the charge of a static polaron $Q_0^p = e n_0$. In $(CH)_x$ $n_0 = 1$ and Q= e, i.e., we have the excitation with the standard relation of charge (-e) and spin (1/2) corresponding to the usual polaron. In the case of the moving polaron and in the limit $\beta^2 \ll 1$ an additional term proportional to β^2 appears

$$Q_\infty^p = Q_0^p + \delta Q_\infty^p, \qquad (6)$$

where $\delta Q^p_\infty = \beta^2 \frac{en}{2} \frac{\Delta_0 - K_0 V_F}{\Delta_0 + K_0 V_F}$. When $\omega_0 \to 0$ we have that $K_0 V_F \to \Delta_0$ and $\delta Q^p_\infty \to 0$ in accordance with the result for the kink where no correction terms proportional to β^2 appear in the limit $W \to \infty$ for the charge of the excitation state. In $(CH)_x$ the level ω_0 is fixed $\omega_0 = K_0 V_F = \frac{\Delta_0}{\sqrt{2}}$ so that $\delta Q^p_\infty \simeq 0{,}17 e \beta^2$.

Consider now the correction terms proportional to δ. From eq.(5) we obtain

$$Q^p = Q^p_0 + \delta Q^p_{st} + \delta Q^p_d \,, \tag{7}$$

where $\delta Q^p_{st} = \frac{4n K_0 V_F}{\pi W} e$ and $\delta Q^p_d = \delta Q^p_\infty + \frac{n\beta^2}{2} \delta Q^p_{st}$.

When $\omega_0 \to 0$ we have $\delta Q^p_{st} \to 2\delta Q^s_{st}$ in accordance with the fact that in this limit the polaronic state "decays" into an infinitely far appart kink-antikink pair state. In $(CH)_x$ $\delta Q^p_{st} \simeq 0.09 e$.

We calculate the energy of the polaron excitation in the model and obtain the result

$$E_p = \frac{2n}{\pi} \frac{K_0 V_F}{\sqrt{1-\beta^2}} \{1 + \frac{\omega_0 (1-\beta^2)}{K_0 V_F [1+\beta^2 (\frac{K_0 V_F}{\omega_0})^2]} \operatorname{arctg} \frac{\omega_0}{K_0 V_F} \} \tag{8}$$

$$+ \frac{2K_0 V_F \beta^2}{\pi \lambda \sqrt{1-\beta^2}} + (n_0 - n \;) \omega_0 \,.$$

Taking into account only correction terms proportional to β^2 we get from (8)

$$E_p = \frac{2n}{\pi} [K_0 V_F + \omega_0 \operatorname{arctg} \frac{\omega_0}{K_0 V_F}] + (n_0 - n) \omega_0 + \tag{9}$$

$$+ \beta^2 \{ \frac{n}{\pi} (K_0 V_F) [1 - 3 (\frac{\omega_0}{K_0 V_F}) \operatorname{arctg} \frac{\omega_0}{K_0 V_F}] + \frac{2K_0 V_F}{\pi \lambda} \}.$$

The last term in (9) determines the dynamical contribution to the polaron mass. In $(CH)_x$ we have

$$E_p = \frac{2\sqrt{2}\,\Delta_0}{\pi} + \frac{\sqrt{2}\,\Delta_0}{\pi} [1 - \frac{3\pi}{4} + \frac{1}{\lambda}] \beta^2 \,, \tag{10}$$

where the first term corresponds to the energy of creation of the static polaron whereas the second term gives the dynamical correction to the polaron mass $\delta M_p = \frac{2\sqrt{2}\,\Delta_0}{\pi V_F^2}(1 - \frac{3\pi}{4} + \frac{1}{\lambda}) \approx 0{,}37 M_p$, where M_p is obtained from the kinetic term in the Hamiltonian and has a value $M_p \simeq 1{,}3\, m_e$. Thus, the effect of the polaron motion gives rise to a considerable contribution to the polaron mass.

In conclusion we note that the obtained results have a great importance in describing the electrical and transport properties of the trans-$(CH)_x$ chains as well as in relativistic quantum field theory where the dynamical masses of solitons appear due to motion.

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