

## Long-Range Order in Quasi-One-Dimensional Conductors

S. N. Artemenko<sup>1,2,\*</sup> and Thomas Nattermann<sup>2</sup>

<sup>1</sup>*Institute for Radioengineering and Electronics of Russian Academy of Sciences, Mokhovaya strasse 11-7, Moscow 125009, Russia*

<sup>2</sup>*Institute für Theoretische Physik, Universität zu Köln, Zùlpicher Strasse 77, 50937 Köln, Germany*

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We study the formation of the charge-density wave long-range order in a system of repulsive 1D electrons coupled to 3D phonons. We show that the charge-density wave can be stabilized by interaction with phonons in quasi-1D crystals and semiconducting nanowires. In the case of metallic atomic chains, interaction with phonons of a 3D substrate is not enough, and violation of the translational invariance by commensurable perturbation or disorder is needed. The possibility of stabilization of superconductivity in 1D electrons with attraction by means of tunnel coupling to a 3D metal is considered.

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The basic electronic properties of three-dimensional (3D) solids are usually well described within Landau's Fermi-liquid picture, including phase transitions into symmetry-broken states like the superconducting (SC) or charge-density wave (CDW) state. Even in cases where the bare interaction is not weak, energy and momentum conservation reduce the relevant part of the phase space making a perturbative approach possible. This is *not* the case in 1D systems where interaction is always strong. Single-electron quasiparticles do not exist; the only low energy excitations are charge and spin collective modes. Such a state is called the Luttinger liquid (LL) (for a review see Ref. [1]). A peculiarity of 1D systems is that long-range order (LRO) cannot exist [2]. In practice, however, 1D systems are embedded in a 3D world which results in the coupling of 1D electrons to substrates, gates, etc. Such systems are quasi-1D rather than purely 1D systems. Then LRO and phase transitions into symmetry-breaking states are not excluded.

It was shown recently [3] that interaction of 1D electrons with 3D metallic gate can lead to quantum phase transitions and to a power-law decay of the order parameter at zero temperature. We will show below that coupling to 3D environment can result in phase transitions and true LRO even at *finite* temperatures. Different realizations of the 1D electrons embedded in 3D environment will be considered. The first one is a semiconductor-based quantum wire in which dimensionality of the conduction electrons is reduced by dimensional quantization. Such wires typically have a diameter of the order of 10 nm; hence they contain thousands of primitive cells in the cross section perpendicular to the wire [4]. The phonon system in such wires can be considered to be effectively 3D. Then electron-phonon coupling can result in the CDW LRO, and we will determine the conditions under which it will occur. Such CDW state is different from the states characterized by quasi-LRO close to a 1D Wigner crystal [5,6] expected in 1D quantum wires with long-range Coulomb interaction.

Another interesting class of quasi-1D conductors are highly anisotropic 3D crystals with chainlike structure.

These materials exhibit commonly metallic behavior and transitions to symmetry-broken states described in terms of Fermi-liquid ideas. For instance, inorganic quasi-1D metals like blue bronzes, NbSe<sub>3</sub>, etc. undergo Peierls' transitions to a CDW state. LL in such metals is not formed because of the instability towards Fermi-liquid behavior around the Fermi energy in the presence of small interchain hopping integral  $t_{\perp} \ll E_F$  [7]. In the same time interchain coupling makes them three-dimensional and provides possibility of LRO. Whereas the main properties of quasi-1D conductors at higher temperatures are well understood, at low temperatures they demonstrate many intriguing properties which are not yet explained convincingly, e.g., the anomalous behavior of the dielectric function interpreted as a new glassy phase [8]. Furthermore, a transition to a low temperature state characterized by LL-like conductivity was detected in focused-ion beam processed crystals [9]. In order to account for such behavior the possibility of stabilization of the LL state by defects in quasi-1D metals was considered [10], but electron-phonon coupling and the formation of CDWs was not taken into account. Though formation of LL in quasi-1D metals is problematic because of the instability towards Fermi-liquid behavior, LL-like behavior is expected to be seen if  $t_{\perp}$  is small compared to the other energy scales of the system related, e.g., to disorder or to energy gap in the spectrum. The formation of a CDW energy gap can indeed result from the coupling of the quasi-1D crystals electrons to 3D phonons, as will be studied below. We also consider a strictly 1D electronic system interacting with 3D phonons of a substrate (e.g., chain of metallic atoms or a single-wall nanotube). We find that in this case the violation of the translational invariance is needed to stabilize the CDW LRO. Such a violation can be induced by commensurability effects or disorder in the substrate.

So far we considered repulsive interaction between electrons. In the opposite case of attractive interaction, we find that in quasi-1D systems like 1D semiconducting nanowires or quasi-1D crystals, the SC LRO can be stabilized by coupling to a normal 3D metal, while in case of strictly

1D electronic system this can be performed by a tunnel contact with a superconductor.

For brevity we consider first repulsive spinless electrons exhibiting a 1D spectrum described by the Tomonaga-Luttinger model. Further below we will include the modifications due to electron spin and the long-range nature of the Coulomb interaction. The electrons are assumed to be coupled to 3D phonons. The system is then described by an action  $S = S_{\text{el}} + S_{\text{ph}} + S_{\text{el-ph}}$  consisting of the electronic, the free-phonon part and the electron-phonon interaction, respectively.  $S_{\text{el}}$  can be expressed in bosonized form in terms of the displacement field  $\Phi_\rho(\tau, x, \mathbf{n})$ , where  $x$  and  $\tau$  denote space and imaginary time, and  $\mathbf{n}$  the chain index, respectively [11]:

$$S_{\text{el}} = \sum_{\mathbf{n}} \int dx d\tau \frac{1}{2\pi v_F} [(\partial_\tau \Phi_\rho)^2 + v_\rho^2 (\partial_x \Phi_\rho)^2]. \quad (1)$$

Here  $v_\rho = v_F/K_\rho$  is the velocity of plasmons,  $v_F$  the Fermi velocity, and  $K_\rho$  the LL parameter measuring the strength of the interaction:  $K_\rho < 1$  for repulsive and  $K_\rho > 1$  for attractive interaction. Sum over  $\mathbf{n}$  represents summation over conducting chains of quasi-1D crystal or over elementary cells for semiconductor quantum wire, say, in Wannier representation.

Free phonons are described by the elastic displacement field  $\varphi$  with a harmonic action

$$S_{\text{ph}} = \frac{S}{2} \int \frac{d^3 q}{(2\pi)^3} d\tau [(\partial_\tau \varphi)^2 + \omega_{\text{ph}}^2(\mathbf{q}) \varphi^2]. \quad (2)$$

Here  $S$  is the cross-section area of the primitive cell in the perpendicular plane,  $\omega_{\text{ph}}^2(\mathbf{q}) = c_\parallel^2 q_\parallel^2 + c_\perp^2 \mathbf{q}_\perp^2$ . We need to keep only slowly varying part of the  $2k_F$  component of the displacement field leading to the CDW transition; therefore, in most of the cases the weak dependence of  $\omega_{\text{ph}}(\mathbf{q})$  on  $q_\parallel$  can be neglected. Finally, the electron-phonon part reads

$$S_{\text{el-ph}} = \frac{\gamma}{\pi\alpha} \sum_n \int dx d\tau [\varphi e^{2i\Phi_\rho} + \varphi^* e^{-2i\Phi_\rho}], \quad (3)$$

where  $\gamma$  is the electron-phonon coupling constant.

A similar action was used by Voit and Schulz [12] in the study of electron-phonon interaction in 1D conductors. They found modifications of the electron spectrum and the phonon dynamics, but no true LRO was present in the purely 1D case considered by them. To solve the problem for the case of 3D phonons we follow Voit and Schulz and integrate out phonon degrees of freedom. This leaves the effective action  $S_{\text{eff}} = S_{\text{el}} + S_{\text{int}}$  with

$$S_{\text{int}} = -\frac{1}{2} \left( \frac{\gamma}{\pi\alpha} \right)^2 \sum_{n, n_1} \int dx d\tau d\tau_1 D_\varphi(\tau - \tau_1, n - n_1) \times \cos[2\Phi(\tau, x, n) - 2\Phi(\tau_1, x, n_1)], \quad (4)$$

where  $D_\varphi$  is the free-phonon propagator, and its Fourier transform reads  $D_\varphi(\omega, \mathbf{q}_\perp) = [\omega^2 + \omega_{\text{ph}}^2(\mathbf{q}_\perp)]^{-1}$ .

Next we consider the diagrammatic series for correlation function  $D_\rho(\tau, x, \mathbf{n}) = \langle \Phi_\rho(\tau, x, \mathbf{n}) \Phi_\rho(0, 0, 0) \rangle$ . It can be found in a standard way in terms of free correlation function  $D_\rho^{(0)}$  and mass operator  $\Sigma$ .

$$D_\rho^{-1} = (D_\rho^{(0)})^{-1} - \Sigma, \quad D_\rho^{(0)} = \pi v_F / (\omega^2 + q_\parallel^2 v_\rho^2). \quad (5)$$

We calculate  $\Sigma$  in the lowest approximation in electron-phonon coupling, and find

$$\Sigma = \delta(x) \left( \frac{\gamma}{\pi\alpha} \right)^2 \left[ D_\varphi(\tau, n) e^{-2(D_\rho(0,0) - D_\rho(\tau, n))} - \delta(\tau) \delta(\mathbf{n}) \times \int d\tau_1 \sum_{n_1} D_\varphi(\tau_1, n_1) e^{-2(D_\rho(0,0) - D_\rho(\tau_1, n_1))} \right]. \quad (6)$$

It is not simple to solve Eq. (6) in general case, but we can solve it in an interesting limiting case when temperature and phonon frequencies are small compared to electronic energies. Note that if we neglect fluctuations of the displacement field  $\varphi$  then the action Eq. (1) and (3) reduces to that of the sine-Gordon model. For  $K_\rho < 1$  the latter describes the state with the excitations spectrum characterized by a finite dynamic mass  $M$  [1]. So we expect that the mass operator must yield a mass  $M$  in the denominator of the correlation function  $D_\rho$  (5) at frequencies  $\omega \sim M \gg \omega_{2k_F} = c_\parallel(2k_F)$ . On the other hand, according to the form of Eq. (3) the mass operator must vanish in the limit  $\omega, \mathbf{q}_\perp \rightarrow 0$ . So we seek  $\Sigma(\omega, q_\perp)$  in the form

$$\Sigma(\omega, q_\perp) = -\frac{M^2}{\pi v_F} \frac{(\omega^2 + c_\perp^2 q_\perp^2)}{(\omega^2 + c_\perp^2 q_\perp^2 + \zeta M^2)}, \quad (7)$$

and assume that the parameters to be found,  $\zeta$  and  $M$ , satisfy conditions  $\zeta \propto (\omega_{2k_F}/M)^2 \ll 1$ . Combining Eqs. (5) and (7) we obtain the correlation function

$$D_\rho = \frac{\pi v_F (\omega^2 + c_\perp^2 q_\perp^2 + \zeta M^2)}{(\omega^2 + \omega_1^2)(\omega^2 + \omega_2^2)}. \quad (8)$$

The poles of the denominator describe two eigenmodes instead of a single mode only in Ref. [12], the number of modes corresponding to number of variables,  $\Phi_\rho$  and  $\varphi$ ,

$$\omega_1^2 \approx M^2 + q_\parallel^2 v_\rho^2, \quad \omega_2^2 \approx c_\perp^2 q_\perp^2 + \frac{\zeta M^2 q_\parallel^2 v_\rho^2}{M^2 + q_\parallel^2 v_\rho^2}. \quad (9)$$

The mode  $\omega_1$  is related mainly to electronic fluctuations, while the soft mode  $\omega_2$  mainly controls phase fluctuations of the new Peierls-deformed lattice, i.e., of the CDW. Note that the infrared divergence in  $\langle \Phi_\rho^2 \rangle = \int \frac{d\omega}{2\pi} \frac{S d^3 q}{(2\pi)^3} D_\rho(\omega, \mathbf{q})$  is removed now and the expectation values of the  $2k_F$  component of the electronic density are finite

$$O_{\text{CDW}} = \frac{\langle e^{2i\Phi_\rho} \rangle}{2\pi\alpha} = \frac{1}{2\pi\alpha} \left( \frac{M}{\Lambda v_\rho} \right)^{K_\rho}. \quad (10)$$

So using Eq. (8) in (6) we find that the mass operator has indeed the form (6) provided  $K_\rho$  is not too close to 1 (i.e., for strong enough electron-electron repulsion) and

$$T, \omega_{2k_F} \ll M, \quad \ln \frac{\Lambda v}{M} \gg \sqrt{\zeta} \ln \frac{c_{\parallel} k_F \sqrt{S}}{c_{\perp}}, \quad (11)$$

with values of parameters

$$M = 2\Lambda v_F \left( \frac{\sqrt{2\lambda} K_\rho}{\alpha \Lambda} \right)^{1/(1-K_\rho)}, \quad \zeta = \frac{\omega_{2k_F}^2}{M^2}, \quad (12)$$

where  $\lambda = \frac{2\gamma^2}{\pi v_F \omega_{2k_F}^2} \ll 1$  is dimensionless electron-phonon coupling constant, and  $\Lambda \approx 1/\alpha$  is a large momentum cutoff. The last relation in Eq. (11) is easily satisfied if the anisotropy of the phonon spectrum is not too large but cannot be satisfied in case of 1D phonon spectrum.

When this result is applied to quasi-1D crystals there is another mechanism of three dimensionality, namely, interchain tunneling that could lead to instability of the LL behavior. However, in the presence of finite mass  $M$  induced by coupling to phonons contribution of the interchain hopping can be neglected provided the interchain coupling is small enough.

The same results can be obtained by neglecting fluctuations of the amplitude of the  $2k_F$ -displacement field,  $\varphi = \eta e^{i\chi}$ , and using the self-consistent harmonic approximation (SCHA) [1]. In this way one can calculate  $\langle \chi^2 \rangle$

$$\langle \chi^2 \rangle = \begin{cases} 2\sqrt{\zeta} K_\rho \int \frac{S d^2 q_{\perp}}{(2\pi)^2} \frac{\omega_{2k_F}}{\omega_{\text{ph}}} \mathbf{K} \left( \frac{\omega_{2k_F}}{\omega_{\text{ph}}} \right) & \text{at } T \ll \omega_{\text{ph}}, \\ \pi K_\rho \sqrt{\zeta} \int \frac{S d^2 q_{\perp}}{(2\pi)^2} \frac{T \omega_{2k_F}}{c_{\perp} q_{\perp} \omega_{\text{ph}}} & \text{at } T \gg \omega_{\text{ph}}, \end{cases} \quad (13)$$

where the elliptic integral  $\mathbf{K} \left( \frac{\omega_{2k_F}}{\omega_{\text{ph}}} \right) \approx \ln \left( \frac{4\omega_{2k_F}}{c_{\perp} q_{\perp}} \right)$  for  $q_{\perp} \rightarrow 0$ . Thus CDW phase fluctuations,  $\langle \chi^2 \rangle$ , are small under conditions (11). If we neglect small value  $\langle \chi^2 \rangle$  then our problem is reduced to the exactly solved sine-Gordon and massive Tiring models [1,12]. The value of  $M$  (12) agrees with these models deep in the massive region (when interaction is strong enough). For noninteracting electrons,  $K \rightarrow 1$ , the exact solutions yield the result of the classical Peierls theory  $M \sim \Lambda v_F e^{-(1/\lambda)}$ .

A finite value of the order parameter in Eq. (10) follows from dependence of the mass operator (7) on  $q_{\perp}$ . In a strictly 1D electronic system interacting with 3D phonons of a substrate the dependence on  $q_{\perp}$  is absent and  $\Sigma = 0$  at  $\omega$ ,  $q_{\perp} \rightarrow 0$ . This is because the phase fields  $\Phi$  or  $\chi$  themselves do not couple to physical fields in a translationally invariant system. Indeed, in the limit  $\omega$ ,  $q \rightarrow 0$  they describe translations of the electrons and the lattice, respectively, as a whole. The physical fields are related to time and spatial derivatives of the phase fields. Hence

phase fluctuations cannot diffuse into 3D space effectively because their interaction with 3D phonons disappears in the infrared limit. Therefore, the contribution of the mode  $\omega_2$  to  $\langle \chi^2 \rangle$  remains divergent and coupling to 3D phonons does not lead to LRO similar to results of Refs. [12]. To remove the infrared divergence in  $\langle \chi^2 \rangle$  one needs to break the translational invariance, e.g., by a commensurate potential in the substrate or by disorder.

Let us first consider the violation of translational invariance by a potential with period  $\pi/k_F$  along the  $x$  direction. The additional contribution to the action,

$$\delta S = Y \sum_n \int dx d\tau [O_{2k_F}^* \varphi(n) + O_{2k_F} \varphi^*(n)], \quad (14)$$

is presented in a form resembling the electron-phonon interaction (3). Here  $O_{2k_F}$  describes density perturbations,  $O_{2k_F} = |O_{2k_F}| \exp(i2k_F x + i\chi_0)$ , inducing a potential,  $Y O_{2k_F}$ , that acts on  $2k_F$  phonons.

Taking into account that destruction of the LRO is controlled by phase fluctuations one can neglect fluctuations of the amplitude of the phonon field [12]. Then using the SCHA we integrate out the electronic degrees of freedom and the phonon operators at all chains except the metallic one,  $\varphi(n=0) = \eta e^{i\chi}$ . This results in an effective action for the CDW phase

$$\delta S_{\text{eff}} = Y \int dx d\tau |O_{2k_F}| \eta \cos(\chi - \chi_0). \quad (15)$$

With Eq. (15) the results for single metallic chain become similar to (12) and (13) if we substitute  $c_{\perp}^2 q_{\perp}^2 \eta^2$  by  $Y |O_{2k_F}| \eta$ . Then instead of Eq. (13) we obtain

$$\langle \chi^2 \rangle \sim K_\rho \sqrt{\zeta} \ln \left( \frac{\gamma \lambda^{K_\rho/2(1-K_\rho)}}{Y |O_{2k_F}| \sqrt{S}} \right).$$

In the limit of small commensurate potential,  $Y \ll \gamma$  or  $O_{2k_F} \sqrt{S} \ll 1$ , the logarithm can be large. However, even in this case  $\langle \chi^2 \rangle$  can be small due to the small factor  $\sqrt{\zeta}$ .

The divergence in  $\langle \chi^2 \rangle$  can be removed also by disorder. In this case one has to substitute  $O_{2k_F}$  in Eq. (14) by the local impurity potential in the substrate  $V(r) = \sum_i V \delta(r - r_i)$ . This leads to a term similar to Eq. (15) but with  $\sum_i \delta(x - x_i) \cos(\chi - 2k_F x_i)$  replacing  $\cos(\chi - \chi_0)$ . Though this will remove the divergence in  $\langle \chi^2 \rangle$  due to quantum fluctuations, true LRO is not expected since the latter is destroyed by the disorder. Nevertheless, for weak disorder the phase coherence length will be quite large as it is in CDW conductors.

For system of spinful electrons the results are qualitatively similar to the spinless case. The spin is taken into account by adding to Eq. (1) a spin term analogous to the charge one [1]. The electron-phonon term (3) also must be modified [12]; namely, the integrand is multiplied by  $\cos \sqrt{2} \Phi_\sigma$  where  $\Phi_\sigma$  is the spin phase field, and factors 2 in the exponents are substituted by  $\sqrt{2}$ . After going through

the same steps as in the spinless case we find mass operators for correlation functions  $D_\rho$  and  $D_\sigma$ . For the charge sector  $\Sigma_\rho$  has a form similar to Eq. (7), while  $\Sigma_\sigma$  is not dispersive, so the spin excitations are described by dispersion relation similar to  $\omega_1$  (9) but with different velocity. The masses for charge and spin sectors are equal in the main approximation

$$M = \Lambda v_F [\lambda K_\rho^{K_\rho} K_\sigma^{K_\sigma} / (\alpha \Lambda)^2]^{1/(2-K_\rho-K_\sigma)}. \quad (16)$$

Since we consider repulsive electrons we can ignore the backscattering in the interaction. While in case of interelectronic attraction it leads to the spin-gapped Luther-Emery phase (cf. [1]), in our problem it results only in small corrections.

Up to now we considered the short-range interaction and treated  $K_\rho$  as a constant. In the case of Coulomb interaction it depends on wave vector. The exact form of  $K_\rho(\mathbf{q})$  depends on crystal structure, but in the long-wavelength limit one can describe interaction by the Fourier transform of the Coulomb potential. Then  $K_\rho^2(\mathbf{q}) = (1 + \kappa^2/q^2)$ , where  $1/\kappa$  is Thomas-Fermi screening length. This results in qualitative modifications of the spectrum of the eigenmodes. Inserting  $v_\rho = v_F/K_\rho$  into (9) we find that the mode  $\omega_1$  approaches at  $q_\perp = 0$  the plasma frequency, and the phason mode  $\omega_2$  is not a soft mode anymore. Similar hardening occurs in the LL density mode without the coupling to phonons [11] and in the CDW phase mode in classical Peierls theory [13].

Similar to the CDW case, but with action written in terms of dual field  $\Theta_\rho$  [1], one can study stabilization of SC LRO in a 1D electronic system with attraction, ( $K_\rho > 1$ ). Since the SC phase is conjugate to the particle number operator and the fixed number of particles makes fluctuations of the phase infinite, one can try to let the particle number to fluctuate in order to diminish fluctuations of the SC phase by coupling to a normal or SC 3D metal via a tunnel junction providing a way to transfer fluctuations of the phase to 3D space. We describe the coupling to the 3D metal by a tunnel Hamiltonian. The 3D metal is presented by the BCS Hamiltonian in the Bogolyubov self-consistent approximation. Then we integrate out the fermions of the 3D metal and obtain an effective action describing coupling to the SC order parameter,  $\Delta$ , of the 3D metal:

$$S_{\text{tun}}^{(\text{eff})} = \sum_n \int dx d\tau i (e^{2i\Theta} \Delta + e^{-2i\Theta} \Delta^*). \quad (17)$$

We describe  $\Delta$  by a Ginzburg-Landau free energy for a 3D superconductor with critical temperature  $T_c$ . So we consider coupling to a superconductor for  $T < T_c$ , and to a normal metal for  $T > T_c$ . We find that the SC LRO can be stabilized by coupling to a normal 3D metal in quasi-1D structures where dependence of  $\Theta_\rho$  on transverse coordinates is possible. In strictly 1D systems, coupling to a

normal metal does not stabilize the LRO, and only quantum phase transitions as discussed in Ref. [3] are possible. This happens because, like in the CDW case, physical fields are related to derivatives of the SC phase, and coupling to 3D space vanishes in the infrared limit. So, again, the symmetry breaking is needed. The symmetry is violated if the 3D metal is in the SC state,  $\langle \Delta \rangle \neq 0$  in Eq. (17), and the problem is reduced to the sine-Gordon model. Hence, the LRO becomes possible.

In conclusion, we found that coupling of electrons in quasi-1D systems to 3D objects should lead to symmetry-breaking transitions described in terms of the LL ideas. The transition to the CDW state was studied in case when phonon frequency is much smaller than typical electronic energy and the repulsion between electrons is strong enough. Both conditions are satisfied in quasi-1D crystals where typical values of the Peierls gap are above 500 K, and the interaction parameter  $K_\rho$  is quite small,  $K_\rho \sim 0.1-0.3$  [10]. Our study of the SC transition explains possibility of the LRO formation in quasi-1D systems but it has more model character because we consider electronic attraction as granted and do not study mechanism of attraction.

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\*art@cplire.ru

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