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## Coulomb screening in quasi one-dimensional conductors. II. Bosonization method

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**Résumé.** — Nous étudions le modèle de Tomonaga pour un système de chaînes parallèles avec les interactions de Coulomb de longue portée, en utilisant la méthode de bosonisation. Les rôles respectifs de l'interaction écrantée à longue portée et de l'interaction nue à portée intermédiaire sont examinés dans la fonction de corrélation  $2k_F$  CDW/SDW. Nous obtenons l'expression complète pour cette fonction dans la limite du couplage faible.

**Abstract.** — The Tomonaga model for a system of parallel chains with the long range Coulomb interactions is investigated by the bosonization technique. The respective rôles of the screened long range and the bare intermediate range interactions are examined in the  $2k_F$  CDW/SDW correlation function. The accurate expression for this latter function is derived in the weak-coupling limit.

It is now well established that the results obtained on the one dimensional models with short-range on-chain interactions bear relevance for the understanding of the phase transitions in some quasi one-dimensional conductors [1]. This stimulated the attempts to give a clear physical interpretation to the effective couplings which appear in the one-dimensional theories. In particular it turned out [2] that the attention should be given to the reduction of the long range intra and interchain Coulomb forces to the effective on-chain coupling constants. Recently, one of us approached [3] this problem by the summation of the parquet diagrams, using the RPA screened forward scattering and neglecting the backward interchain coupling [3] (henceforth referred to as paper I). The main complications appeared in the forward, Tomonaga [4], part of the diagrammatic approach. This led us to investigate the corresponding Tomonaga

model, using the bosonization method [5] in parallel with the diagrammatic summation. The bosonization is one among several techniques [6] which in principle can give the exact solution of this model. We shall use it here to determine the  $2k_F$ -CDW/SDW correlation function in the weak-coupling limit, adding this piece of knowledge to the already existing expressions for the long-wavelength CDW spectrum and the electron self-energy [7]. The bosonization was previously used [5, 6] to solve the Tomonaga model with the constant forward coupling and our approach represents a physically interesting generalization of these results to the case of long-range interactions. Our results support and complement those obtained in I by the parquet summation.

As in I we shall consider the system of equivalent parallel conducting chains which are regularly spaced in a square array, with lattice constants  $d_{\parallel}$  and  $d_{\perp}$ .

Interchain hopping and electron-electron interaction *via* phonons are neglected i.e. only the forward Coulomb intrachain and interchain interactions are assumed to be important. We are concerned with the long range interactions which are correctly described in the point charge approximation. The corresponding Coulomb matrix element multiplied by the density of states per atom and spin,  $\eta_F = d_{\parallel}/2 \pi \hbar v_F$  is

$$v\alpha_c,$$

where

$$\alpha_c \approx \sum_{\mathbf{g}} \frac{4\pi}{d_{\perp}^2 |q^2 + (\mathbf{q}_{\perp} + \mathbf{g})^2|}$$

$$v = \frac{e^2}{2\pi\hbar v_F} = n_F \frac{e^2}{d_{\parallel}}. \quad (1)$$

Here  $\mathbf{g}$  is the transverse reciprocal lattice vector;  $q$  is the component of the wave vector along the chain,  $\mathbf{q}_{\perp}$  is the component perpendicular to the chain axis in the first Brillouin zone of transverse reciprocal space.

In order to study the rôle of the strong singularity (1), which falls in the region of forward scattering processes assuming that  $k_F > d_{\perp}^{-1}$  (cf. I), we write the Hamiltonian  $H$  in terms of the density operators [5, 6]

$$\begin{aligned} \hat{H} = 2\pi\hbar v_F \left\{ \frac{1}{L} \sum_{q>0} \int \frac{d_{\perp}^2 d\mathbf{q}_{\perp}}{4\pi^2} [\hat{\rho}_1(-q, -\mathbf{q}_{\perp}) \hat{\rho}_1(q, \mathbf{q}_{\perp}) + \hat{\rho}_2(q, \mathbf{q}_{\perp}) \hat{\rho}_2(-q, -\mathbf{q}_{\perp})] + \right. \\ \left. + \frac{1}{L} \sum_{q>0} \int \frac{d_{\perp}^2 d\mathbf{q}_{\perp}}{4\pi^2} v\alpha_c [\hat{\rho}_1(-q, -\mathbf{q}_{\perp}) \hat{\rho}_1(q, \mathbf{q}_{\perp}) + \hat{\rho}_2(q, \mathbf{q}_{\perp}) \hat{\rho}_2(-q, -\mathbf{q}_{\perp}) \right. \\ \left. + \hat{\rho}_1(-q, -\mathbf{q}_{\perp}) \hat{\rho}_2(q, \mathbf{q}_{\perp}) + \hat{\rho}_1(q, \mathbf{q}_{\perp}) \hat{\rho}_2(-q, -\mathbf{q}_{\perp})] \right\}. \quad (2) \end{aligned}$$

Here  $\rho_{1,2}(q, \mathbf{q}_{\perp})$  are the usual Fourier transforms of  $\hat{\rho}_{1,2}(q, l)$  the density operators for the electrons on the chain with index  $l$ .  $L$  is the length of the chain and integration over  $\mathbf{q}_{\perp}$  is to be taken in the first Brillouin zone. In the Hamiltonian (2) we have omitted the constant terms which are irrelevant for subsequent calculations. Specific features of the Tomonaga model are that

- i) the Hamiltonian is bilinear in the density operators  $\hat{\rho}_1(q, \mathbf{q}_{\perp})$  and  $\hat{\rho}_2(q, \mathbf{q}_{\perp})$ ,
- ii) spectrum of the free system is assumed linear in  $q$ , and independent of  $\mathbf{q}_{\perp}$ ,
- iii) the following commutation relations are valid

$$\begin{aligned} [\hat{\rho}_1(-q, -\mathbf{q}_{\perp}), \hat{\rho}_1(q', \mathbf{q}'_{\perp})] &= -q \frac{L}{2\pi} N \delta_{q,q'} \delta_{\mathbf{q}_{\perp}, \mathbf{q}'_{\perp}} \\ &\quad (q, q' > 0) \\ [\hat{\rho}_2(-q, -\mathbf{q}_{\perp}), \hat{\rho}_2(q', \mathbf{q}'_{\perp})] &= q \frac{L}{2\pi} N \delta_{q,q'} \delta_{\mathbf{q}_{\perp}, \mathbf{q}'_{\perp}} \\ [\hat{\rho}_1(q, \mathbf{q}_{\perp}), \hat{\rho}_1(q', \mathbf{q}'_{\perp})] &= [\hat{\rho}_2(q, \mathbf{q}_{\perp}), \hat{\rho}_2(q', \mathbf{q}'_{\perp})] \\ &= [\hat{\rho}_1(q, \mathbf{q}_{\perp}), \hat{\rho}_2(q', \mathbf{q}'_{\perp})] = 0 \end{aligned} \quad (3)$$

( $N$  is the number of chains in the system).

By the straightforward generalization of the usual procedure [6, 8] the Hamiltonian (2) can be diagonalized by the unitary transformation  $\exp \hat{S}$ , where

$$\hat{S} = \frac{2\pi}{L} \int \frac{d_{\perp}^2 d\mathbf{q}_{\perp}}{4\pi^2} \sum_{q>0} \frac{\phi(q, \mathbf{q}_{\perp})}{q} [\hat{\rho}_1(-q, -\mathbf{q}_{\perp}) \hat{\rho}_2(q, \mathbf{q}_{\perp}) - \hat{\rho}_1(q, \mathbf{q}_{\perp}) \hat{\rho}_2(-q, -\mathbf{q}_{\perp})]$$

and

$$\phi(q, \mathbf{q}_{\perp}) = -\frac{1}{4} \ln(1 + 2v\alpha_c). \quad (4)$$

The resulting plasmon spectrum of the system is [7, 9]

$$\hbar\omega_p(q, \mathbf{q}_{\perp}) = \hbar v_F q(1 + 2v\alpha_c)^{1/2}. \quad (5)$$

The characteristic wave vector in equations 4 and 5 is the Thomas-Fermi value  $k_{TF}^2 = 8\pi v/d_{\perp}^2$ . For  $|\mathbf{q} + \mathbf{q}_{\perp}| < k_{TF}$  the plasmon has strong anisotropic three-dimensional dispersion. For  $|\mathbf{q} + \mathbf{q}_{\perp}| > k_{TF}$  this dispersion merges into the usual acoustic-like dispersion  $v_F q$  familiar from the constant-interaction theories [6].

A suitable method of calculating the response functions of the Tomonaga model is based upon the boson representation of fermion fields [5]. Following Luther and Peschel these operators can be bosonized as follows

$$\hat{\psi}_{1,2}(\mathbf{r}_p, x) \leftrightarrow \frac{e^{\pm ik_F x}}{\sqrt{2\pi\alpha}} \exp \left\{ \frac{\pm 2\pi}{L} \sum_{k>0} \frac{e^{-\frac{\alpha}{2}k}}{k} [\hat{\rho}_{1,2l}(k) e^{ikx} - \hat{\rho}_{1,2l}(-k) e^{-ikx}] \right\} \equiv \hat{O}_{1,2l}(x),$$

where  $\alpha$  is the cut-off parameter of the bosonization. In order to calculate explicitly the CDW/SDW susceptibility for  $|k| \simeq 2k_F$  at  $T = 0$  which is defined by  $i\chi_{ij}(x, t) = \theta(t) \langle 0 | [\hat{\psi}_1^+(\mathbf{r}_i, x, t) \hat{\psi}_2(\mathbf{r}_j, x, t), \hat{\psi}_2^+(\mathbf{r}_j, 0, 0) \hat{\psi}_1(\mathbf{r}_i, 0, 0)] | 0 \rangle$ , where  $|0\rangle$  is the exact ground state of the system and field operators are in Heisenberg picture, the boson representations  $\hat{O}_{1l}(x), \hat{O}_{2l}(x)$  of the field operators  $\hat{\psi}_1(\mathbf{r}_p, x), \hat{\psi}_2(\mathbf{r}_p, x)$  are used. Following further Luther and Peschel we obtain after a lengthy but straightforward calculation

$$i\chi_{ij}(x, t) = \frac{e^{-i2k_F x}}{(2\pi\alpha)^2} \theta(t) \cdot \{ \exp[F_{ij}^{(1)}(x, t) + F_{ij}^{(2)}(x, t)] - \exp[F_{ij}^{(1)*}(x, t) + F_{ij}^{(2)*}(x, t)] \}. \quad (6)$$

Here

$$F_{ij}^{(1,2)}(x, t) = \int_0^\infty \frac{dq}{q} \int \frac{d^2q_\perp}{4\pi^2} (e^{-\frac{\alpha}{2}q} + e^{\phi(q, \mathbf{q}_\perp)} - 1)^2 \cdot (e^{\pm i\mathbf{q}_\perp \cdot (\mathbf{r}_j - \mathbf{r}_i) \mp i(qx \pm \omega_F(q, \mathbf{q}_\perp)t)} - 1) \quad (7)$$

and  $\phi, \omega_p$  are given by (4) and (5) respectively. It can be easily shown that the integrals in (7) are divergent ( $-\infty$ ) for  $0 < |\mathbf{r}_i - \mathbf{r}_j| < k_{TF}^{-1}$  due to the contribution of the  $q^2 + q_\perp^2 > k_{TF}^2$  integration range. On physical grounds we can thus conclude that the susceptibility (6) is diagonal in the chain indices [8]. The physical content of the  $i = j$  functions  $F(x, t)$  can be seen from the following representation

$$\cos \omega_p \left( \frac{x}{u} \pm t \right) - 1 = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{(v_F q)^2 \sin \omega \left( \frac{x}{u} \pm t \right)}{\omega(\omega^2 - v_F^2 q^2)} \cdot \frac{\omega^2 - v_F^2 q^2}{\omega^2 - \omega_p^2} \frac{\omega_p^2}{(v_F q)^2} d\omega$$

where  $u = v_F(1 + 2v\alpha_c)^{1/2}$ . The dielectric function of the Tomonaga model

$$\epsilon_T(q, \mathbf{q}_\perp; \omega) = \frac{\omega^2 - \omega_p^2}{\omega^2 - v_F^2 q^2}$$

appears explicitly here and the functions (7) contain the screened Coulomb interaction. This agrees with the use of this interaction in I. For further analysis it is thus convenient to follow I and divide the transverse reciprocal space into three regions

- i) region  $B_1$  :  $q^2 + q_\perp^2 > k_{TF}^2, q < k_{TF}$
- ii) region  $B_2$  :  $q^2 + q_\perp^2 > k_{TF}^2, q > k_{TF}$
- iii) region  $S$  :  $q^2 + q_\perp^2 < k_{TF}^2, q < k_{TF}$ .

In the regions  $B_1$  and  $B_2$  the dielectric function is approximately equal to unity, that is, the interaction is bare in these regions. In the region  $S$  (« screened region ») the interaction is either statically or dynamically screened.

Expanding in terms of small  $v$  the contributions to the functions (7) of the regions  $B_1$  and  $B_2$  are respectively

$$F_{B_1}^{(1,2)} = \int_0^{k_{TF}} \frac{dq}{q} \left( (1 - v) e^{-\alpha q} - 2v \exp\left(-\frac{\alpha}{2}q\right) \log \frac{\epsilon_F}{\omega_0} \right) \cdot (e^{\pm i(qx \mp v_F q t)} - 1) \quad (7a)$$

$$F_{B_2}^{(1,2)} = \int_{k_{TF}}^\infty \frac{dq}{q} \left( e^{-\alpha q} - 2v \exp\left(-\frac{\alpha}{2}q\right) \log \frac{\epsilon_F}{v_F q} \right) \cdot (e^{\pm i(qx \mp v_F q t)} - 1) \quad (7b)$$

where  $v = \frac{d_\perp^2}{4\pi}(k_{TF}^2 - q^2)$ ,  $\epsilon_F = v_F k_F \sim v_F \frac{\pi}{d_\parallel}$  and  $\omega_0 = v_F k_{TF}$  is the maximum three-dimensional plasma frequency [9]. The functions (7a, b) are Lorentz invariant (i.e. depend on  $x \pm v_F t$ ) due to the fact that in the regions  $B_1$  and  $B_2$  the spectrum  $\omega_p$  is a linear function of momentum i.e.  $\omega_p \approx v_F q$ .

In order to calculate contributions of the region  $S$  to the functions (7) we transform the integration over  $q_\perp^2$

into the integration over  $\omega_p \approx \frac{\omega_0 q}{(q^2 + q_\perp^2)^{1/2}}$ . Integrating by parts in the region defined above and retaining the leading, Lorentz invariant term we obtain

$$F_S^{(1,2)} \approx \int_0^{k_{TF}} \frac{dq}{q} \left( v e^{-\alpha q} - \eta v \exp\left(-\frac{\alpha}{2} q\right) \right) (e^{\pm i(qx \mp v_F q t)} - 1), \quad (7c)$$

where  $\eta$  is a constant of the order of unity ( $\eta \approx 1$ ).

We proceed by treating separately the contributions to  $F$  [1, 2] from  $B_1$  and S and from  $B_2$ . They dominate at large and intermediate distances and times respectively. Adding (7a) to (7c) and performing the integrations over  $q$  we obtain, using equation 6, the susceptibility for  $d_{1,2} = |x \pm v_F t| > k_{TF}^{-1}$

$$i\chi(x, t) \approx \frac{e^{-i2k_F x}}{4\pi^2} \theta(t) \cdot \alpha^{-2v(2\log_{\omega_0} \frac{\varepsilon_F}{\omega_0} + 1)} \cdot \{ [(d_1 - i\alpha)(d_2 + i\alpha)]^{v(2\log_{\omega_0} \frac{\varepsilon_F}{\omega_0} + 1) - 1} - [(d_1 + i\alpha)(d_2 - i\alpha)]^{v(2\log_{\omega_0} \frac{\varepsilon_F}{\omega_0} + 1) - 1} \}. \quad (8)$$

Fourier transforming (8) at  $|k| = 2k_F$  and taking the limit  $\omega \rightarrow 0$ , a well known [5, 6] singularity of the power law type is recovered

$$\chi(\omega) \sim \omega^{-v(2\log_{\omega_0} \frac{\varepsilon_F}{\omega_0} + 1)}. \quad (9)$$

The first term in the exponent of (9) comes from the region  $B_1$  and agrees with the result of I. This term dominates in the weak coupling limit  $\omega_0 \ll \varepsilon_F$  ( $v \ll 1$  and/or  $d_\perp \gg d_\parallel$ ). The second term of the exponent in (9) is provided by the screening range and becomes relevant on approaching the intermediate couplings  $\omega_0 \lesssim \varepsilon_F$  ( $v \lesssim 1$ ,  $d_\perp \gtrsim d_\parallel$ ). Although it was possible in I to estimate roughly this contribution by the diagrammatic analysis, the present approach shows that the contribution of the screened range S can be exponentiated in the correlation function. This in spite of the fact found in I that the contribution of S to ladder diagrams is much smaller than to the mixed diagrams, relative to the constant interaction case. This means that the mixed diagrams dominate the correlations in both cases. On the other hand they are particularly sensitive [10] to the transverse hopping  $t_\perp$ , neglected here by assumption (ii). The result (9) is thus restricted to  $\omega > t_\perp$ . Further on,  $B_1$  and S contribute the terms of the same sign to the exponent. The screening thus does not result in an effective attractive interaction although it reduces considerably the bare interaction (1). The superconductivity requires other mechanism than Coulomb interaction even in one dimension ( $\omega > t_\perp$ ).

Next we calculate the contribution of the region  $B_2$ . For this purpose it is convenient to replace  $\exp\left(-\frac{\alpha}{2} q\right) \log \frac{\varepsilon_F}{v_F q}$  by the modified Bessel function  $K_0(q/k_F)$  on noting that the bosonization method requires [11]  $\alpha \lesssim k_F^{-1}$ . In such a way the logarithmic singularity at small  $q$  is properly treated and the integrations are easier to perform. With  $q > k_{TF}$  (i.e.  $q^2 + q_\perp^2 > k_{TF}^2$ ) we obtain the following expression for the susceptibility at  $k_{TF}^{-1} > |d_{1,2}| > k_F^{-1}$

$$i\chi(x, t) = \frac{e^{-i2k_F x}}{4\pi^2} \theta(t) \cdot \exp[v \log^2(k_F d_1 + \sqrt{k_F^2 d_1^2 + 1}) + v \log^2(k_F d_2 + \sqrt{k_F^2 d_2^2 + 1})] \times \left[ \frac{e^{i\phi_x}}{(d_1 - i\alpha)(d_2 + i\alpha)} - \frac{e^{-i\phi_x}}{(d_1 + i\alpha)(d_2 - i\alpha)} \right] \quad (10)$$

where  $\phi_x = v\pi \log \frac{k_F d_1 + \sqrt{k_F^2 d_1^2 + 1}}{k_F d_2 + \sqrt{k_F^2 d_2^2 + 1}}$ .

When calculating the Fourier transform of the susceptibility at  $|k| = 2k_F$  we encounter the integrals of the type

$$\int_1^\infty \frac{dz}{z} e^{v \log^2 z} \cdot \exp\left(i \frac{\omega}{2\varepsilon_F} z\right)$$

$$\int_1^\infty \frac{dz}{z} \log z \cdot e^{v \log^2 z} \cdot \exp\left(i \frac{\omega}{2\varepsilon_F} z\right),$$

with  $z = k_F |d_1| \approx k_F |d_2|$ . The singular part of the Fourier transform of the susceptibility is thus determined essentially by

$$\int_1^{\left(\frac{\omega}{2\varepsilon_F}\right)^{-1}} \frac{e^{v \log^2 z}}{z} dz, \quad \int_1^{\left(\frac{\omega}{2\varepsilon_F}\right)^{-1}} \frac{e^{v \log^2 z}}{z} \log z dz.$$

The asymptotic expression of the susceptibility for  $\omega_0 < \omega < \varepsilon_F$  is in consequence

$$\chi(\omega) \rightarrow \frac{1}{2 \pi v_F} \frac{\log \frac{1}{2} \frac{\omega}{2 \varepsilon_F}}{4 v \log^2 \frac{\omega}{2 \varepsilon_F}} \cdot \left(\frac{\omega}{2 \varepsilon_F}\right)^{-2v \left|\log \frac{\omega}{2 \varepsilon_F}\right|} \quad (11)$$

It shows a power law singularity with the power which itself is logarithmically singular. The result (11), was first obtained by means of the bosonization method (cf. Ref. 22 of I) and agrees with the calculations made in I by the diagrammatic technique.

In summary the results of the bosonization method agree with the results of the diagrammatic summation. Moreover, the bosonization method is simpler and allows us to derive the more precise expressions for the  $2 k_F$  CDW correlation function, which extrapolate better towards the intermediate couplings. This improvement is obtained at the expense of the backward scattering, which is neglected in the Tomonaga model. As to the physical relevance of such results, the TTF-TCNQ family seems to be closest to the limit of large forward scattering [12, 1].

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