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Ionic plasma screening and long-range electron correlations in quasi-one-dimensional conductors

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ABSTRACT

In quasi-one-dimensional systems with the intercalation-type doping, the dynamical response of dopant ions can substantially affect the interplay of density-wave and superconducting instabilities. A generic model system of Coulombically coupled Luttinger-liquid chains augmented by the interaction with the ion displacements is exactly solved in the forward-scattering channel providing for the resulting system excitations and electron correlations. For a jellium-like ion response, the effect of the bare electron–electron repulsion is essentially canceled by the ions. Superconducting correlations can then be developed due to a non-polarizational interaction with an additional phonon mode.

Ever since the original Little's suggestion [1] of the exciton-mediated superconductivity in specially designed macromolecules, the physics of one-dimensional (1D) and quasi-1D conductors has been a subject of extensive research that uncovered a rich area of interactions-driven competing instabilities in these systems (see, e.g., Refs. [2–8] for reviews). With modern progress in nanoscience, the search for quasi-1D superconductivity is continuing in materials quite different from those envisioned by Little, such as in bundles of carbon nanotubes. It has been argued [9], e.g., that substitutional doping of carbon nanotubes could lead to an increase of the superconducting (SC) transition temperature followed by experiments [10,11] claiming an onset of superconductivity at 15 K (see a recent report [12] and references therein for other experimental and theoretical developments).

Intercalation-type doping is an important practical means of providing the electronic subsystem with (extra) charge carriers without disrupting its chemical-bond skeleton. For quasi-1D systems, this doping is, for instance, a major route for controlling electric properties of conducting polymers [13]. High dopant concentrations may be achieved in different ways: by traditional chemical volume doping [13] or by interfacial double layer charging [14], particularly with ionic liquids [15,16]. Many intercalation-doped systems exhibit qualitatively new properties such as superconductivity in graphite compounds [17,18], in fullerides [19] and in hydrocarbons [20]. In addition to supplying charge carriers, dopant ions and intercalants in general may however also play other roles. So the size of the dopant is known to critically affect the distance between the fullerene molecules in alkali-doped fullerides [19]. Electron coupling with intercalant vibrations was attributed to be the reason for higher SC transition temperatures in certain graphite compounds [21] as well as in fullerides [22].

In this Letter we want to emphasize the role of the collective dynamics of dopant ions for quasi-1D electronic conductors as a source of the ensuing long-range electron–ion Coulomb interaction, similarly to how it occurs in 3D for the BCS model [3,23,24]. We point out that the dynamical response of the dopants may radically affect the interplay of the interactions by effectively screening the long-range electron–electron repulsion and thereby creating more favorable conditions for SC correlations. This represents another example of strong effects that may take place upon embedding 1D electronic systems in 3D environments [25].

Our demonstration is based on the model of an anisotropic 3D system of Coulombically-interacting parallel Luttinger-liquid chains introduced by Schulz [4,26] that will be supplemented by their Coulomb coupling to the ionic subsystem. Being interested only in the spin-independent long-range Coulomb interactions, we limit our discussion here to the Coulomb forward-scattering processes with small momentum transfer $\mathbf{q}$ ($g_2 = g_4$ processes in the g-ology language [4,5,26]), for which the macroscopic expression for the bare Coulomb interaction

$$V_0(\mathbf{q}) = 4\pi/q^2, \qquad q^2 = q_x^2 + q_\perp^2, \tag{1}$$

is valid. Here the 3D momentum ($\hbar = 1$) $\mathbf{q} = (q_x, \mathbf{q}_\perp)$ is specified via its components along, q_x, and perpendicular, $\mathbf{q}_\perp$, to the chains. When screened by high-frequency dielectric polarization modes, the Coulomb interaction becomes [26]

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$$V(\mathbf{q}) = \frac{4\pi}{\varepsilon_{\parallel} q_x^2 + \varepsilon_{\perp} q_{\perp}^2}, \tag{2}$$

allowing for anisotropy of the background dielectric constants $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$.

The electronic part H_e of the electron–ion system Hamiltonian

$$H = H_e + H_i + U_{ei} \tag{3}$$

has been treated by Schulz [26]. Using the standard bosonization method [4–6], it can be written as

$$H_e = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + U_{ee}, \tag{4}$$

where electron–electron repulsion

$$U_{ee} = \frac{e^2}{2\mathcal{V}} \sum_{\mathbf{q}} V(\mathbf{q}) \rho_e(-\mathbf{q}) \rho_e(\mathbf{q}) = \frac{\omega_p^2}{16\pi v_F} \sum_{\mathbf{q}} |q_x| V(\mathbf{q}) B_{\mathbf{q}}^{\dagger} B_{\mathbf{q}}, \tag{5}$$

is determined by electron densities $\rho_e^{\dagger}(\mathbf{q}) = \rho_e(-\mathbf{q})$ and further expressed via bosonic charge density operators [6]

$$b_{\mathbf{q}} = (b_{\mathbf{q}\uparrow} + b_{\mathbf{q}\downarrow})/\sqrt{2}$$

and their combinations

$$B_{\mathbf{q}} = b_{\mathbf{q}} + b_{-\mathbf{q}}^{\dagger}.$$

The spin density fluctuations are not interacting in this model and do not need to be considered explicitly (that would correspond to a term like the first term in Eq. (4)). Featured in Eqs. (4) and (5) are the non-interacting electron energies

$$\epsilon_{\mathbf{q}} = v_F |q_x|, \tag{6}$$

volume $\mathcal{V}$ of the system and the bare electronic plasma frequency $\omega_p^2 = 4\pi n_e e^2/m$, that is convenient to use to quantify the 3D electron concentration n_e. All Hamiltonians in this Letter are assumed to be normally ordered, which is not shown explicitly.

Standard [5,6] exact diagonalization of the electronic Hamiltonian (4) by the Bogoliubov boson transformation [27] then results in

$$H_e = \sum_{\mathbf{q}} E_0(\mathbf{q}) c_{\mathbf{q}}^{\dagger} c_{\mathbf{q}},$$

$c_{\mathbf{q}}$ being the boson operators of the plasmon excitations with the anisotropic dispersion

$$E_0^2(\mathbf{q}) = \epsilon_{\mathbf{q}}^2 + \left(\frac{q_x}{q}\right)^2 \omega_p^2(\mathbf{q}), \tag{7}$$

where

$$\omega_p^2(\mathbf{q}) = \omega_p^2 \frac{V(\mathbf{q})}{V_0(\mathbf{q})}.$$

Except for the gapped uniform plasmon mode with $\mathbf{q}_{\perp} = 0$, the spectrum (7) exhibits a gapless acoustic $E_0(\mathbf{q}) \propto |q_x|$ behavior at $q_x \to 0$, see Fig. 1. The velocities of these modes are higher than v_F with the ever increasing values towards smaller $q_{\perp}^2$. The result of the long-range electron–electron repulsion therefore is the enhanced "tendency towards density-wave ordering, whereas the superconducting fluctuations are suppressed" [26].

In the context of our further discussion, it is instructive to recognize that the spectrum (7) can be immediately derived as corresponding to the zeroes, $\varepsilon_e(E_0, \mathbf{q}) = 0$, of the frequency ω and momentum $\mathbf{q}$-dependent dielectric function

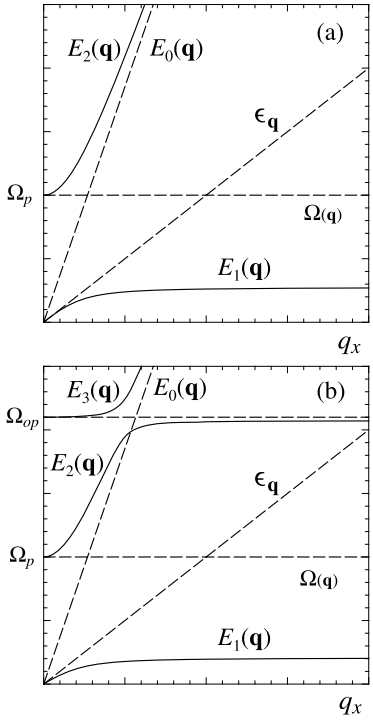

Fig. 1. Illustration of the dispersion of elementary excitations as a function of q_x for a fixed value of $q_{\perp}$ in systems of: (a) electrons plus jellium-like dopant ions; (b) electrons plus jellium-like dopant ions plus one non-polarizational dispersionless optical phonon mode of energy Ω_{op}. The results shown here are calculated with the bare Coulomb interaction, $V(\mathbf{q}) = V_0(\mathbf{q})$, and $\omega_p/\Omega_p = 50$. Note that the values of system parameters for *illustrative* plots in this Letter have been chosen just to assist in a better visual display of the discussed qualitative features. Solid lines are used to show the resulting excitation branches, and dashed lines are for various "contributing" excitations as indicated, including non-interacting electron (6), purely electronic plasmon (7) and phonon (11) spectra.

$$\varepsilon_e(\omega, \mathbf{q}) = 1 + \left(\frac{q_x}{q}\right)^2 \frac{\omega_p^2(\mathbf{q})}{\epsilon_{\mathbf{q}}^2 - \omega^2} \tag{8}$$

reflecting the fact that the electrons can move only along the x-axis. The dielectric functions we consider here refer to the renormalization of the electric potentials [3,6] and are related to the generalized dielectric tensor [28] $\varepsilon_{ij}(\omega, \mathbf{q})$ as $\varepsilon = \varepsilon_{ij} q_i q_j / q^2$.

We restrict our explicit treatment of the ionic subsystem here to the case of the ionic "jellium" [23,24]. Only longitudinally polarized displacements of the ions contribute to the macroscopic charge densities and need to be considered; the ionic subsystem excitations in Eq. (3) are thus represented as a collection of longitudinal phonons:

$$H_i = \sum_{\mathbf{q}} \Omega(\mathbf{q}) a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}}. \tag{9}$$

In the jellium model, the kinetic energy of ions is augmented only by the ion–ion Coulomb repulsion:

$$U_{ii} = \frac{e^2}{2\mathcal{V}} \sum_{\mathbf{q}} V(\mathbf{q}) \rho_i(-\mathbf{q}) \rho_i(\mathbf{q}) = \frac{\Omega_p^2}{16\pi} \sum_{\mathbf{q}} \frac{q^2}{\Omega(\mathbf{q})} V(\mathbf{q}) A_{\mathbf{q}}^{\dagger} A_{\mathbf{q}}, \tag{10}$$

where ionic densities $\rho_i^{\dagger}(\mathbf{q}) = \rho_i(-\mathbf{q})$ and $A_{\mathbf{q}} = a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}$ are combinations of the phonon operators. The bare ionic plasma frequency $\Omega_p^2 = 4\pi n_i e^2/M$ is convenient to use in Eq. (10) to quantify the 3D ion concentration n_i (singly-charged ions of mass M). Note that the electron n_e and ion n_i concentrations need not be equal