Charge ordering in quasi-one-dimensional systems with frustrating interactions

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Motivated by the co-existing charge and spin order found in strongly correlated ladder systems, we study an effective pseudospin model derived from an earlier work [12], we will explore the scenario of $U_\perp \gg V$ in an earlier work [12], we will explore the scenario of $U_\perp \ll V$ below. In the spin sector, coupling between the two systems leads to a $S = 1/2$ Heisenberg ladder-type model, and has been studied extensively by several authors [13]. Interchain spin coupling turns out to be relevant, opening up a spin gap concomitantly with generating AF/dimer ordered ground states with spontaneously broken SU(2)/translation symmetries.

We now analyse the charge sector. To begin, we introduce (bond-)fermion operators via a Jordan-Wigner transformation. In terms of these fermions, upon denoting the chains as $a = \uparrow, \downarrow$, we find an effective Hamiltonian for the 1D Hubbard model with an equal-spin pairing term and an on-site spin-flip term

$$H = -\sum_{j,a} [2t \tau_{j,a}^{\pi} + V \tau_{j,a}^{\pi} \tau_{j+1,a}^{\pi}]$$

where $2t$ is the transverse field, $V$ is the n.n interaction pseudospin coupling. Here, the $\tau$ represent charge degrees of freedom in an effective model derived from a more basic electronic Hamiltonian for a 1/4-filled system [6, 7, 8]. This is the 1D Ising model in a transverse field.

$$H = -\sum_{j,a} [2t \tau_{j,a}^{\pi} + V \tau_{j,a}^{\pi} \tau_{j+1,a}^{\pi}] + \sum_{j,a} [\psi_{j,a} \psi_{j+1,a}^{\dagger} + h.c.] + U \sum_{j,a} \sum_{\alpha=\uparrow,\downarrow} \langle \psi_{j,a}^{\dagger} \psi_{j,a} \rangle$$

$$+ \sum_{j,a} \mu \langle \psi_{j,a}^{\dagger} \psi_{j,a} \rangle$$

where $\mu$ is the chemical potential, $U$ is the on-site (Hubbard) interaction parameter, and $\tilde{V} = V/4$ the pairing strength. Note that while we treat the parameters $\tilde{t}$ and $\tilde{V}$ as independent parameters for the sake of generality, $\tilde{t} = V = V$ in our original model.
where $\Pi_\rho \rightarrow \Pi_\rho / v_\rho$ and spin $\sigma \rightarrow \sigma$ variables, we obtain the effective low-energy bosonic Hamiltonian

$$H = \frac{1}{2\pi} \int dx [v_\rho K_\rho (\pi \Pi_\rho (x))^2 + \frac{v_\rho}{K_\rho} (\partial_x \phi_\rho (x))^2]$$

$$+ \frac{1}{2\pi} \int dx [v_\sigma K_\sigma (\pi \Pi_\sigma (x))^2 + \frac{v_\sigma}{K_\sigma} (\partial_x \phi_\sigma (x))^2]$$

$$+ \frac{U_\rho}{2\pi \alpha} \int dx \cos (\sqrt{8} \phi_\rho) + \frac{U_\sigma}{2\pi \alpha} \int dx \cos (\sqrt{8} \phi_\sigma)$$

$$+ \frac{\tilde{V}}{2\pi \alpha} \int dx \cos (\sqrt{2} \phi_\rho) \cos (\sqrt{2} \phi_\sigma) - \frac{\sqrt{2} \mu}{\pi} \int dx \partial_x \phi_\rho (x)$$

$$+ \frac{t_\perp}{\pi \alpha} \int dx \cos (\sqrt{2} \phi_\rho) \cos (\sqrt{2} \phi_\sigma) + \frac{V_1}{\pi \alpha} \int dx \cos (\sqrt{8} \phi_\sigma)$$

$$+ \frac{V_2}{\pi \alpha} \int dx \cos (\sqrt{2} \phi_\rho) \cos (\sqrt{2} \phi_\sigma) + \frac{V_4}{\pi \alpha} \int dx \cos (\sqrt{8} \phi_\rho) \quad (4)$$

where $\Pi_\rho = \frac{1}{\pi} \partial_x \theta_\rho \ , \ \Pi_\sigma = \frac{1}{\pi} \partial_x \theta_\sigma \ , \ v_\rho K_\rho = v_\rho \sigma , v_\sigma K_\sigma = v_\sigma \rho$ and $v_\rho / K_\rho = v_\rho (1 + \sqrt{2} / \pi \nu_\rho)$ and $v_\sigma / K_\sigma = v_\sigma (1 - \frac{\nu_\sigma}{\pi \nu_\rho})$. Among the various cosine potentials, we have the usual spin-flip backscattering $\cos (\sqrt{8} \phi_\sigma)$ and Umklapp $\cos (\sqrt{8} \phi_\rho)$ terms as well as the triplet superconducting $\cos (\sqrt{2} \phi_\rho) \cos (\sqrt{2} \phi_\sigma)$ term. The chemical potential term can be absorbed by performing the shift $\phi_\rho \rightarrow \phi_\rho + \sqrt{2} K_\rho \mu / \hbar \tilde{\sigma}$. The cosine potentials with couplings $V_1, V_2$ and $V_4$ are generated under RG by the $t_\perp$ and $\tilde{V}$ terms. We find the RG equations for the various couplings to second-order as

$$\frac{dU_\rho}{dt} = (2 - 2 K_\rho) U_\rho$$

$$\frac{dU_\sigma}{dt} = (2 - 2 K_\sigma) U_\sigma - \frac{1}{K_\sigma} - K_\rho t_\perp$$

$$\frac{d\tilde{V}}{dt} = (2 - \frac{1}{K_\rho} - \frac{1}{K_\sigma} + \frac{1}{K_\rho}) \tilde{V} - K_\sigma t_\perp V_2$$

$$\frac{dt_\perp}{dt} = (2 - \frac{1}{K_\sigma} + \frac{1}{K_\rho}) t_\perp - \frac{\tilde{V} V_2}{K_\rho} (K_\sigma U_\sigma + \frac{V_1}{K_\sigma})^2 t_\perp$$

$$\frac{dV_1}{dt} = (2 - \frac{2}{K_\sigma}) V_1 + \frac{1}{K_\rho} - K_\sigma t_\perp$$

$$\frac{dV_2}{dt} = (2 - \frac{2}{K_\sigma}) V_2 - \frac{t_\perp \tilde{V}}{K_\sigma}$$

$$\frac{dV_4}{dt} = (2 - \frac{2}{K_\rho}) V_4 \quad . \quad (5)$$

The RG equations for the two interaction parameters $(K_\rho, K_\sigma)$ as well as the parameter $\delta = K_\rho \mu / \nu_\rho$ are found to be

$$\frac{dK_\rho}{dt} = - K_\rho^2 U_\rho^2 + V_1^2$$

$$\frac{dK_\sigma}{dt} = - K_\sigma^2 U_\sigma^2 J_0 (\delta) \alpha$$

$$\frac{d\delta}{dt} = \delta (l) - U_\rho^2 J_1 (\delta) \alpha \ , \quad (6)$$

where $\delta (l) = \delta (l)$, $\alpha$ is a short-distance cut-off like the lattice spacing and $J_0(x), J_1(x)$ are Bessel functions.

For repulsive interactions $(U_\perp > 0)$ between bon-fermions, the $\sigma$ sector is massless and $K_\rho$ flows under RG to the fixed point value $K_\rho^* \gtrsim 1$ and $1/2 \leq K_\rho \leq 1$. At 1/2-filling (for the bond-fermions), the couplings $U_\rho, \tilde{V}, t_\perp, V_1$ and $V_2$ are all relevant while $U_\sigma$ and $V_3$ are irrelevant. The competition to reach strong-coupling first is, however, mainly between $U_\rho, t_\perp$ and $\tilde{V}$. We show below the phase diagram as derived from this analysis.

![FIG. 1: The RG phase diagram in the $(K_\rho, K_\sigma)$ plane for repulsive interchain interactions $(U_\perp < 0)$. The three regions $K_\rho < (1/4(K_\rho + 1/K_\sigma), 1/4(K_\rho + 1/K_\sigma))$, $1/K_\rho > K_\rho > 1/4(1/K_\rho + 1/K_\sigma)$ and $K_\rho > (1/K_\rho, 1/4(K_\rho + 1/K_\sigma))$ give the values of $(K_\rho, K_\sigma)$ for which the couplings $U_\rho, t_\perp$ and $\tilde{V}$ respectively are the fastest to grow under RG.](image)
This gapless phase is the analog of the “Floating Phase” found in the phase diagram of the 1D axial next nearest neighbour Ising model \( \mathbb{P} \). We present in Fig. 2 below a RG flow phase diagram which is projected onto the \((V_1, t_\perp)\) plane (a similar RG flow diagram is found for the case of the anisotropic Heisenberg model in a magnetic field \( h \) \( \mathbb{H} \) in the \((a, h)\) plane, where \( a \) is the anisotropy parameter).

![Figure 2](image)

**FIG. 2**: The RG phase diagram in the \((V_1, t_\perp)\) plane. The thick line characterises the set of points which flow to the intermediate fixed point \((V'_1, t'_\perp)\) shown by the filled circle. The thin lines show all RG flows which flow towards strong-coupling in the two phases \( \mathbb{I} \) and \( \mathbb{II} \), characterised by the relevant couplings \( \tilde{V} \) and \( t_\perp \) respectively.

The regions \( \mathbb{I} \) and \( \mathbb{II} \) characterise all RG flows which do not flow to the intermediate fixed point at \((V'_1, t'_\perp)\). In region \( \mathbb{I} \), \( V_1 \) flows to strong-coupling while \( t_\perp \) decays; for \( 1/2 < K_\rho < 1 \) and \( K_\sigma > 1 \), we know from the above discussion that in this region, the coupling \( \tilde{V} \) will reach strong-coupling first. In region \( \mathbb{II} \), both \( t_\perp \) and \( V_1 \) grow under RG, with the coupling \( t_\perp \) being the first to reach strong-coupling. Thus, the RG trajectory leading to the intermediate fixed point represents a gapless phase separating the two gapped, charge-ordered phases \( \mathbb{I} \) and \( \mathbb{II} \) characterised by the relevant couplings \( \tilde{V} \) and \( t_\perp \) respectively.

For attractive interactions \((U_\perp < 0)\) between the bond-fermions, we can carry out a similar analysis. In this case, we can see that \( K_\rho > 1 \) while \( K_\sigma < 1 \). Then, from the RG equations given above, we can see that the Umklapp coupling \( U_\rho \) and \( V_1 \) are irrelevant while the couplings \( t_\perp, U_\sigma, \tilde{V}, V_2 \) and \( V_3 \) are relevant. The competition to reach strong-coupling first is, however, mainly between \( U_\sigma, t_\perp \) and \( \tilde{V} \). We show below the phase diagram at 1/2-filling for the bond-fermions as derived from this analysis.

In the phase diagram in Fig. 3, the three lines with intercepts at \((K_\rho = 1, K_\sigma = 1)\), \((K_\rho = 1, K_\sigma = 0.64)\) and \((K_\rho = 1, K_\sigma = 1/\sqrt{3})\) are the relations \( K_\sigma = 1/K_\rho \), \( K_\rho = 1/4(1/K_\sigma + 1/K_\rho) \) and \( K_\rho = 1/\sqrt{3} \) respectively.
The regions $K_\sigma < (1/4(K_\sigma + 1/K_\rho), 1/\sqrt{3}, 1/K_\rho > K_\sigma > 1/\sqrt{3}$ and $K_\sigma > (1/K_\rho, 1/4(K_\rho + 1/K_\sigma))$ give the values of $(K_\rho, K_\sigma)$ for which the couplings $U_\sigma, t_\perp$ and $\tilde{V}$ respectively are the fastest to grow under RG.

The regions $K_\sigma < (1/4(K_\sigma + 1/K_\rho), 1/\sqrt{3}, 1/K_\rho > K_\sigma > 1/\sqrt{3}$ and $K_\sigma > (1/K_\rho, 1/4(K_\rho + 1/K_\sigma))$ signify the values of $K_\rho$ and $K_\sigma$ for which $U_\sigma$ (rung-dimer insulator with in-chain Wigner charge-ordering), $t_\perp$ and $\tilde{V}$ (insulator with in-chain dimers and Peierls charge-ordering) respectively are the fastest to reach strong-coupling. This matches our finding of a ground state with in-chain Wigner charge order and rung-dimers in the strongly-coupled ladder with large ferromagnetic rung-couplings in an earlier work [12]. Away from 1/2-filling (for the bond-fermions), depending on which of the three couplings $t_\perp, \tilde{V}$ and $U_\sigma$ is the first to reach strong-coupling, the system exists either as a superconductor with intra-chain hole pairs ($\tilde{V}$) or a superconductor with rung-singlet hole pairs ($U_\sigma$) or a phase reached by following the dominant instability away from the orbital antiferromagnetism like insulating phase ($t_\perp$) but which we are currently unable to describe in greater detail.

To conclude, we have studied a model of strongly correlated coupled quasi-1D systems at 1/4-filling using an effective pseudospin ladder model with $V > t, t_\perp, U_\perp$. Using a bosonisation analysis, we find two different types of charge/spin ordered ground states at 1/4-filling. Transverse bond-fermion hopping is found to stabilise a new, gapped (insulating) phase characterised by interchain two-particle coherence of a type resembling orbital antiferromagnetism [12 13]. The spin fluctuations are described by a $S = 1/2$ Heisenberg ladder-type model for all cases studied here: the spin excitations are always massive. Away from this filling, either intra- or inter-chain superconductivity in a gapped spin background is found to be the stable ground state. We also find the existence of an intermediate gapless phase lying in between two gapped, charge-ordered phases (characterised by the relevant couplings $\tilde{V}$ and $t_\perp$ respectively) in the RG phase diagram of our model. Our analysis is especially relevant to ladder systems like $Sr_{14-x}Ca_xCu_{24}O_{41}$ and $\alpha - NaV_2O_5$ or $\beta - Na_{0.33}V_2O_5$ (a superconductor) which exhibit charge/spin long range order at $x = 0$ and superconductivity beyond under pressure and/or doping [2 12].

SL and MSL thank the DFG (Germany) and EPSRC (UK) respectively for financial support.

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