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# Spin and charge necklaces at commensurate filling

**K Kikoin**[1], **M N Kiselev**[2]

[1] School of Physics and Astronomy, Tel-Aviv University, Tel-Aviv 69978, Israel

[2] The Abdus Salam International Center for Theoretical Physics, Strada Costiera 11, 34014 Trieste, Italy

E-mail: konstk@post.tau.ac.il

**Abstract.** The charge and spin properties of spin chains decorated with dimers and closed trimers (equilateral triangles) with commensurate partial filling (1/4 and 1/3, respectively) are considered. It is shown that due to the charge separation both systems prefer the ground state with even occupation per elementary cell, where the spin spectrum possesses the Haldane gap for negative spin exchange and magnon-like for positive coupling. The charge spectrum is always gapped.

## 1. Introduction

The idea of necklace was introduced in the physics of strongly correlated electron systems in the seminal paper [1], where real 3D Kondo lattices were approximated by a chain of strongly correlated "ions" (sites) characterized by the spin quantum number and a Fermi reservoir was attached to each site. Later on this idea was exploited in the physics of multiterminal quantum dots, where the necklace was attached to a quantum dot in a contact with two electrodes (leads) represented by the Fermi seas of conduction electrons. One may mention for example the studies of singlet-triplet interplay [2] or shot noise in tunneling through a dimer attached to a 1D channel [3], complicated regime of Kondo tunneling through a quantum dot in a form of triangular loop [4] and the studies of the size effects in Kondo screening in a geometry with a stripe attached to a quantum dot [5].

The notion of a necklace is also useful in the theory of quasi 1D chains, where each site is decorated by a finite chain of side sites. The simplest object of this type is a "centipede ladder", where the necklace is formed from dimers [6,7]. One may attach a strip of arbitrary length to each site in a chain. When the length of this strip is infinite, one returns back to the initial idea of Doniach, provided the interaction between electrons occupying these sites is not taken into account.

Another option for further generalization of the initial Doniach's idea is to use closed elements (loops) for spin chain decoration. In this case really new physics arises when the interaction between the electrons within a single loop is strong enough. The simplest decoration element of this kind is a triangle. The quasi-1D chain of triangles ("Heisenberg delta-chain" was introduced in [8], where the frustration effects due to the interplay between the ferro-and antiferromagnetic coupling were studied. The complementary geometry to this delta chain is a chain where each triangle is attached to the chain by one of its apexes. The spin properties of this type of Heisenberg chain was studied in [9]. If all sites of triangle are singly occupied, the spin properties

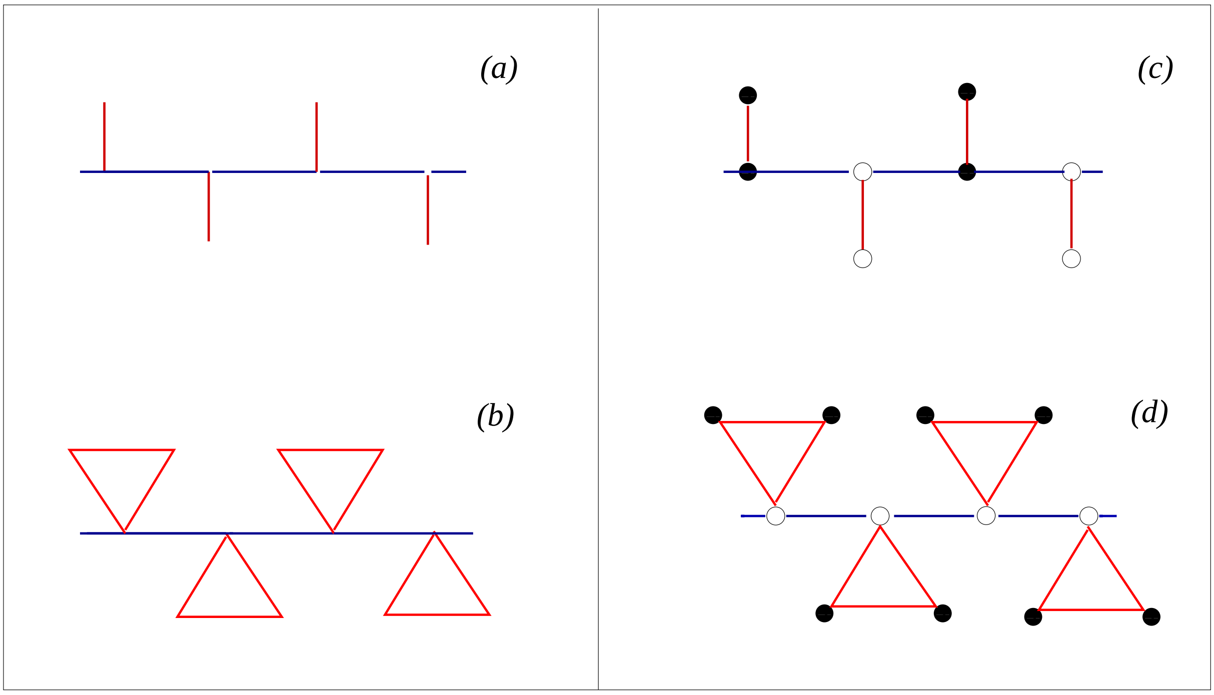


**Figure 1.** (a) Geometry of centipede chain; (b) geometry of triangular necklace; (c) dimerization of centipede chain; (d) charge separation in a triangular necklace. Here the empty and occupied sites are shown by white and black circles.

of triangle are characterized by a chirality $\vec{s}_1 \cdot \vec{s}_2 \times \vec{s}_3$, and the corresponding entanglement affects the ground state of this necklace.

In the present paper we compare the ground states of two types of quantum necklaces with partial filling, namely the quarter filled centipede ladder [7] (Fig. 1a) and one-third filled triangular necklace [9] )(Fig. 1b). We show that both these necklaces with commensurate filling are subject to peculiar dimerization, which results in appearance of energy gaps in charge excitation spectrum while the spin excitation spectrum are gapless for positive effective spin super-exchange or gapped for negative effective coupling.

## 2. Model Hamiltonian and its diagonalization

The geometry of two quantum necklaces under consideration allows various filling of elementary cell [dimer in case (a) and trimer (equilateral triangle) in case (b)]. If each site is occupied by a single electron, one deals with the generalized Heisenberg model with interaction between neighboring spins both along the chain and within a cell. We consider here the commensurate partial filling (one electron per cell or 1/4 filling in case (a) and two electrons (one hole) per cell or 1/3 filling in case (b).

The generic model Hamiltonian is $H = H_r + H_l$, where

$$H_r = \epsilon_0 \sum_{si\sigma} n_{si,\sigma} - t_\perp \sum_i \left( c^\dagger_{\alpha i,\sigma} c_{\beta i,\sigma} + \text{H.c} \right) \tag{1}$$

$$+\frac{1}{2} \sum_{si,\sigma} U n_{si,\sigma} n_{si,\bar{\sigma}} - I_\perp \sum_i \left( \mathbf{s}_{\alpha i} \mathbf{s}_{\beta i} - \frac{1}{4} n_{\alpha i} n_{\beta i} \right),$$

describes the electronic states on the rungs, and

$$H_l = -\left(t_\| \sum_{i\sigma} c^\dagger_{\alpha i,\sigma} c_{\alpha i+1,\sigma} + \text{H.c.}\right) \tag{2}$$

is related to the longitudinal electron hopping along the leg. Here the index $i$ enumerates the elementary cells in the necklace and the indices $\alpha, \beta$ stand for the sites within a given cell $i$. Due to partial filling empty states on the rungs appear and the electron hopping is possible both within a given rung ($t_\perp$) and between neighboring rungs ($t_\|$). We retained here the direct on-rung exchange interaction $I_\perp$, which is supposed to be ferromagnetic.

We consider the case of week longitudinal hopping $t_\| \ll t_\perp$. As was shown in [7], the homogeneous state with equal single electron occupation of each rung of centipede ladder is unstable against dimerization with alternating 2/0 occupation of neighboring rungs (Fig. 1c) provided the exchange energy gain due to the on-rung ferromagnetic exchange $I_\perp$ exceeds the hopping energy $2t_\perp$ within a rang. This means that at

$$I_\perp > 2t_\perp, \quad t_\| \ll I_\perp - 2t_\perp \tag{3}$$

one comes to the dimerized chain with alternating rungs in triplet state $S = 1$ and empty rungs with zero spin instead of effective Heisenberg chain with spin s=1/2 per site. In the homogeneous state the centipede ladder should be charge insulator and possess the gapless spinon-like spectrum in the spin sector. In the dimerized states the even rungs are excluded from the effective spin Hamiltonian, which has the form

$$H_{eff} = H_r - J_\| \sum_i \vec{S}_i \cdot \vec{S}_{i+2}, \tag{4}$$

where $\vec{S}_i$ is the spin 1 vector. The exchange coupling constant is $J_\| = t_\|^4/16\Delta_T^3 > 0$, where $\Delta_T = I_\perp - 2t_\perp$.

Thus we have demonstrated that the problem of quarter-filled CL is mapped onto the familiar problem of spin-one Heisenberg chain with ferromagnetic exchange. Only the odd sites are involved in formation of the gapless spin excitations, which, apparently may be described in terms of the spin-wave theory. The quantum critical point separates the domains with linear Goldstone excitations (spinons) in the homogeneous phase and quadratic magnon-like excitations in the dimerized phase.

As to the charge sector, the elementary excitations above the dimerized ground state are charge-transfer excitons, i.e. the pairs of neighboring sites in (1,1) charge configuration propagating coherently on the background of (2,0,2,0...) configuration. The gap for these excitation is $\Delta_T$.

In case of triangular necklace with 1/3 filling the situation is even more peculiar. The same energy gain arguments show that the energy of a single trimer is minimized when two electrons form a triplet pair, provided $I_\perp > 2t_\perp$ similarly to the dimer case. The spectrum in a charge sector consists of a orbital singlet and orbital doublet [10], with a gap between two states $\Delta_{\text{orb}} = 3t_\perp$. Since the triangular symmetry is broken by the longitudinal hopping $t_\|$, the orbital singlet corresponds to two electron occupying the side sites, whereas the doublet is formed by two linear combinations of two other pairs which involve the apex belonging to the chain. Thus under the condition (3), the minimum energy of the system corresponds to the electron configuration of Fig. 1d.

As a result we came to even more paradoxical situation than in the case of centipede ladder. While in the ground state of the centipede necklace every second rung was empty, *all* chain sites are empty in the ground state of the triangular necklace. The effective spin Hamiltonian for this necklace is again the Heisenberg Hamiltonian for spin S=1, where spin belongs to the triangle as a whole. The indirect longitudinal exchange arises only in the 4-th order in hopping, $J_{\|} \sim t_{\perp}^2 t_{\|}^2/\Delta_{\rm orb}^2 \epsilon_0$. In spite of the partial filling the charge excitations are always gapped. This gap arises because of the orbital splitting. The excitations in the spin sector are controlled by the sign of the super-exchange. The spin gap opens for $J_{\|} < 0$ in accordance with the Haldane conjecture [11].

## 3. Concluding remarks

Decorated chains demonstrate the fascinating variety of spin and charge properties. It was shown before that the spin gap in a spin 1 case of the half-filled centipede ladder belongs to the new universality class which differs from that for Haldane spin 1 chain [6,12], because the effective spin space of the triplet/singlet manifold characterizing the spin excitation has dimension 4 and the symmetry SO(4)instead of usual 3d SO(3) spin space. In case of partial commensurate filling with even occupation of elementary cell, the spin properties are described by the Haldane scenario for negative effective coupling or spin-wave theory for positive exchange, whereas the charge excitations demonstrate peculiar instability against charge separation, which results in insulating state instead of expected metallic state of partially filled effective Hubbard model.

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