Exactly solvable 2D topological Kondo lattice model

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Abstract – As a spin-1/2 Kitaev sublattice interacting with a subsystem of spinless fermions is studied on a honeycomb lattice when the fermion band is half-filled. The model Hamiltonian describes a topological Kondo lattice with the Kitaev interaction, it is solved exactly by reduction to free Majorana fermions in a static Z_2 gauge field. A yet unsolved problem of a hybridization of fermions and local moments in the Kondo lattice at low temperatures is solved in the framework of the proposed model. The Kondo hybridization gap is opened and the system is fixed in insulator and spin insulator states, due to the spin-fermion nature of the gap. We will show that the hybridization between local moments and itinerant fermions should be understood as hybridization between corresponding Majorana fermions of the spin and charge sectors. The RKKI interaction between local moments is not realized in the model, a system demonstrates a “quasi-Kondo” scenario of behavior with realization chiral gapless edge states in topological nontrivial phases. The ground-state phase diagram of the interacting subsystems calculated in the parameter space is rich.

Introduction. – The Kondo lattice problem remains an unsolved problem of strong correlated systems, with interacting delocalized and localized electrons [1–3]. The Kondo lattice Hamiltonian describes conduction electrons interacting with local moments arranged regularly. The Kondo lattice approximation is used for the description of rare-earth and transition compounds. The scenarios of hybridization of electrons and local moments, opening of spin and charge gaps at low temperatures, a formation of large volume of the Fermi surface in the Kondo lattice are still unclear. In the framework of a 1D model of the Kondo lattice Tsvelik has shown that the insulating state forms not due to a hybridization of conduction electrons with local moments, but as a result of strong antiferromagnetic fluctuation [1]. Note that the insulator phase in the state of the Kondo insulator is realized in all compounds with odd number of itinerant electrons per local moment.

The Kondo lattice problem is not reduced to a single-impurity Kondo problem where a local moment is screened at low temperatures by conduction electrons and the ground state of an impurity is a spin-singlet [4,5]. The behavior of the system (the Kondo problem) is defined by the exponentially small scale (the Kondo temperature) in the exchange coupling constant.

We hope to explain the phenomenon of the Kondo lattice in the framework of the model of the proposed topological Kondo lattice. We will call a complex system, which includes interacting spin and fermion subsystems and at least one of them is topological, a Kondo lattice. This class of compounds is now known as topological Kondo insulators. Recent experiment on SmB_6 shown that a phase state of a topological Kondo insulator is realized in SmB_6. The compound SmB_6 attracted now attention due to the anomalous behavior of a residual conductivity at low temperature T ∼ 5–7 K that is characterized by a 3D to 2D crossover of the transport carriers. The intermetallic compound SmB_6 is a strongly correlated insulator with topological states at low temperatures, it is the first candidate of a topological Kondo insulator family [6–11]. According to refs. [12–15], the topological state in SmB_6 is a result of indirect interaction of 5d states via strong spin-orbit coupling and hybridization between itinerant 5d and narrow (localized) 4f electronic states. The topological Kondo insulator is formed via strong interaction of dispersive d- and nondispersive f-electronic bands and hybridization between them. Describing a nondispersive band in the framework of the spin operators the system of strongly correlated fermions can be defined on the topological Kondo lattice and the phase of a topological Kondo insulator is realized as its topological state.

We study a 2D model of the topological Kondo lattice at half-filling and small doping. The model of the topological Kondo insulator is the first example of exact solvable model of a topological Kondo lattice, the exact
solution of the Kondo-like lattice model can also be crucial for understanding the behavior of the Kondo lattice. In the framework of the model we show that the hybridization gaps arise in the state of the Kondo insulator. The physics of the model is surprisingly rich.

Model. – We focus on the 2D model of a spin subsystem interacting via the Kitaev interaction with a subsystem of spinless fermions. The total Hamiltonian

$$\mathcal{H} = \mathcal{H}_s + \mathcal{H}_f + \mathcal{H}_{\text{int}}$$  \hspace{1cm} (1)

describes the spin and spinless fermion sublattices, and the interaction between them. The Hamiltonian of the spin subsystem $\mathcal{H}_s$ is defined on a honeycomb lattice with a spin-$\frac{1}{2}$ on each site and an additional exchange interaction between spins within the $z$-links; it can be written in the framework of the Kitaev model [16] with additional $\bar{z}$-links within the $z$-links,

$$\mathcal{H}_s = \Delta_x \sum_{\langle i,j \rangle^x} \sigma_i^x \sigma_j^x + \Delta_y \sum_{\langle i,j \rangle^y} \sigma_i^y \sigma_j^y$$

$$+ \Delta_z \sum_{\langle i,j \rangle^z} \sigma_i^z \sigma_j^z + I \sum_{\langle i,j \rangle^z} \sigma_i^z \sigma_j^z,$$  \hspace{1cm} (2)

where $\langle i,j \rangle$ is a pair of sites connected by $x$-, $y$-, $z$- and $\bar{z}$-links mentioned right after the pair notation, $\sigma^\gamma_j$ are the three Pauli operators at a site $j$, and $\Delta_\gamma$ are the exchange integrals along all the links of the corresponding direction $\gamma = x, y, z$. The interposed $\bar{z}$-link breaks the $z$-link via the $I \sigma_i^z \sigma_j^z$ exchange interaction (the last term in (2)) with the exchange integral $I$ between spins in two additional sites on the $z$-link (see fig. 1). For convenience, consider $\Delta_\gamma, I > 0$.

For the sublattice of the spinless fermions we will use the following tight-binding model that takes into account

$$\mathcal{H}_f = -i t_1 \sum_{\langle l,m \rangle} \left( a_l^\dagger a_m + a_m a_l \right)$$

$$-i t_2 \sum_{\langle l,m \rangle} \left( a_l^\dagger a_m + a_m a_l \right) + \text{h.c.},$$  \hspace{1cm} (3)

where $a_l^\dagger$ and $a_l$ are the spinless creation and annihilation operators defined on the honeycomb fermion sublattice and satisfying the usual anticommutation relations, $t_1$ is an overlap integral of nearest-neighbor hopping between neighbor sites $\langle l, m \rangle$ from $l$ of the type 2 to $m$ of the type 3, $t_2$ is a clockwise (relatively to a honeycomb) next-nearest-hopping between second-neighbors $\langle l, m \rangle$, $l$ and $m$ range all sites of both type 2 and 3.

The unit cell of the lattice consists of four sites of the spin subsystem (namely 1–4 in fig. 2) and two sites of the fermion subsystem (marked by 2 and 3). The term $\mathcal{H}_{\text{int}}$ is governed by a contact interaction between itinerant states of spinless fermions and spin operators at the sites 2–3 that are interposed into the $z$-links,

$$\mathcal{H}_{\text{int}} = \lambda \sum_l (2n_l - 1) \sigma^y_l,$$  \hspace{1cm} (4)

where $\lambda$ is the coupling parameter, $n_l = a_l^\dagger a_l$, $l$ ranges all pairs of spin and fermion sites, namely 2 and 3 of each cell (see fig. 2).

The Hamiltonian (1) defines an exactly solvable model of a topological Kondo insulator on a honeycomb topological Kondo lattice. The Hamiltonian of the spin sublattice $\mathcal{H}_s$ can be exactly diagonalized using the representation of the Pauli operators in terms of a related set of Majorana fermions $b^\gamma_j$ and $c_j$ with commutation rules

$$\{c_i, c_j\} = 2\delta_{ij}, \quad \{b^\gamma_i, b^{\gamma'}_j\} = 2\delta_{\gamma\gamma'}\delta_{ij}, \quad \{c_i, b^\gamma_j\} = 0,$$

with the substitution $\sigma^\gamma_j = i b^\gamma_j c_j$ [16] ($\gamma = x, y, z$). We introduce two types of Majorana fermions on each site for the sublattice of spinless fermions

$$d_l = a_l + a_l^\dagger \quad \text{and} \quad g_l = \frac{a_l - a_l^\dagger}{i},$$
the Hamiltonian $\mathcal{H}$ can thus be rewritten in the form

$$
\mathcal{H} = -i \sum_{\beta = x,y,z} \sum_{(ij) \beta} A^\beta_{ij} c_i c_j - i t_1 \sum_{(l,m)} d_l d_m - i t_2 \sum_{(l,m)} \nu_{lm} d_l d_m + \lambda \sum_i g_i d_i b_i^\dagger b_i^\vphantom{\dagger},
$$

(5)

where the matrix $A$ consists of $A^x_{ij} = \Delta_x u^x_{ij}$ for the directed links $\gamma = x, y, z$ and $A^y_{ij} = I u^y_{ij}$ for the intercalated $x$-link, $u^x_{ij} = -u^y_{ij} = i b_i^\dagger b_j^\vphantom{\dagger}$ and $\nu_{ij} = \pm 1$ stands for clockwise (anticlockwise) next-neighbour hopping inside a corresponding plaquette.

The physical subspace is defined by the constraint $D_j |\psi\rangle_{\text{phys}} = |\psi\rangle_{\text{phys}}$ with $D_j = b_i^\dagger b_j^\vphantom{\dagger} c_j$. The operator $D_j$ acts as the identity operator on the physical subspace [16], it commutes with the Hamiltonian (5).

The plaquette operator [16]

$$
w_s = \sigma_{x1}^z \sigma_{y2}^y \sigma_{y4}^y \sigma_{y5}^z \sigma_{s2}^y \sigma_{s3}^y \sigma_{s4}^y \sigma_{s5}^z,
$$

is defined by a product of the $u^x_{ij}$ operators around a plaquette $s$, see fig. 1. Operators $u_{ij}^x$ are constants of motion with eigenvalues $\pm 1$. Each plaquette operator $w_s$ has thus two eigenvalues $\pm 1$ and it is interpreted as a magnetic flux through the plaquette $s$. The operators $u_l = i g_l b_l^\dagger$ are the constants of motion with eigenvalues $\pm 1$. Thus, the Hilbert space of states might be split into eigenspaces, where all operators $u_{ij}^x$ and $u_l$ might be replaced with their eigenvalues. The variables $u_{ij}^x$ and $u_l$ are identified with a static $\mathbb{Z}_2$ gauge fields on the bonds. The Hamiltonian (5) is thus reduced to a quadratic form. The itinerant fermions and localized moments reconcile with each other via the hybridization with pairing states of spin-fermion Majorana fermions on the lattice sites.

To solve the model exactly, one converts each vortex sector to free spinless fermions [16]. Numerically, we have computed the ground-state energy of the model for a set of finite-size systems and for a various set of the exchange integrals. In all cases we found that the ground-state energy is minimized by the same uniform flux pattern. The vortex uniform sector with $w_s = 1$ for all plaquette operators $w_s$ is the ground state of the model [16,17]. The model is solved analytically for the uniform configurations, due to the translational invariance of the lattice. We now focus on the vortex-free configuration ($w_s = 1$) for the Hamiltonian $\mathcal{H}$ of the entire system (1). A contact interaction (4) breaks both particle-hole symmetry and time reversal (TR) symmetry of the model Hamiltonian and gives a nontrivial ground-state phase diagram of the system.

**Phase analysis.**

**Noninteracting subsystems.** In the absence of the interaction (4), the system is a sum of two decoupled spin and fermion subsystems. The spinless fermion subsystem is always in a topologically nontrivial phase if $t_1 \neq 0$ and $t_2 \neq 0$ [18,19], its spectrum is gapped, one chiral edge mode is presented, see fig. 3. The phase is characterized by the Chern number $C_{ch}$ of the charge sector, $C_{ch} = \pm 1$ depending on the sign of $t_1/t_2$.

The topological phases of the noninteracting spin subsystem are also associated with the Chern number $C_s$. It is convenient to illustrate the ground-state phase diagram of the spin subsystem using Kitaev’s diagram [16] fig. 4—a section by the plane $\Delta^2_x + I \Delta_x + I \Delta_y = \text{const}$ in coordinates $I \Delta_x$, $I \Delta_y$ and $\Delta^2_z$. There are two topological distinct phases: the topological trivial phase (with gapped states) indexed by $C_s = 0$ and the topological nontrivial phase (with gapless states) with $C_s = 1$ are separated by lines of quantum phase transitions. In the case of noninteracting subsystems, an external magnetic field breaks the TR symmetry of the spin subsystem and opens a gap in the spectrum of the Majorana fermions [16] in the gapless region. The structure of energy levels with edge states in the spin sector is shown in fig. 5 for both phases.

**Phase diagram of interacting subsystems.** Let us consider the adiabatic connection of the subsystems via the interaction (4) and evolution of the ground state of the system along $\lambda$ and $I$ directions. We use the fixed parameters of the Hamiltonian (1) $t_1 = 5$ and $t_2 = 1$ in the case of an anisotropic spin-exchange interaction $\Delta_x = \frac{1}{2}$, $\Delta_y = 2$ and $\Delta_z = 1$ to demonstrate a band structure and edge modes observed in the common case. The spectrum of a noninteracting fermion subsystem is gapped, a noninteracting spin subsystem has a gapless spectrum of the Majorana fermions when $\frac{1}{4} \leq |I| \leq \frac{1}{2}$, otherwise it is gapped. There are six bands, corresponding to six sites per unit cell: two high-energy fermion bands and four low-energy spin bands (see fig. 6). The structure of
Thus, the phase diagram of the model system in the coordinates $(I, \Delta_x, I\Delta_y, \Delta_z^2)$ with an exchange integral satisfying the normalization condition $I\Delta_x + I\Delta_y + \Delta_z^2 = 1$ for arbitrary $t_1, t_2$ and $\lambda$, separate the topological phases with the Chern numbers 1 and 2, as will be shown below. We consider the cases $I = 1$ and $I = \frac{1}{2}$ to illustrate these two scenarios of behavior and investigate peculiarities of the topological states.

Scenario 1. At $I = 1$ and $\lambda \neq 0$ the phase state of the system is characterized by two (spin and fermion) gaps in the excitation spectrum. Calculations of the Chern number and edge states show that $C_{\text{ch}} = 1$ and $C_s = 0$ at $\lambda = 0$, a total Chern number is equal to 1 for arbitrary values of $\lambda$. The structure of edge states depends on a direction of folding: the $y$-direction boundary (fig. 8(a)) performs chiral gapless edge modes specified by the fermion sublattice and thus all low-level excitations are fermionic, while the $x$-direction boundary (fig. 8(b)) performs chiral edge modes crossing the Fermi level three times with excitations of spin type (fig. 8(c)). These edge modes are associated with $C = 1$, but the topological insulator’s behaviors are different: it acts as a fermion topological insulator in the $y$-direction and as a spin topological insulator in the $x$-direction.

The interaction term (4) also directly hybridizes the edge states, therefore the edge states are a result of the total spectrum of the system on the one hand, and they are a result of the direct hybridized interaction on the boundary on the other hand.

Scenario 2. Now consider the second scenario of behavior of the Kondo lattice when the gap closed at $\lambda = 0$ in the spectrum of spin excitations opens for $\lambda \neq 0$, as is shown at $I = \frac{1}{2}$ in fig. 9. At $\lambda = 0$ a spin gap closing makes the topological index $C_s$ ill-defined. Taking into account a magnetic field as a weak disturbance that breaks the TR symmetry of the spin subsystem and opens the gap in the spin sector of the spectrum of Majorana fermions [16], we calculate $C_s$ and the edge states of the spin subsystem. According to the obtained calculations, $C_s = 1$ (the same value as $C_{\text{ch}}$). For $\lambda \neq 0$, the gap opens due to a strong hybridization in the low-energy region of the spectrum even in the absence of an external magnetic field. The total Chern number of the system is equal to two, there are
between excitations in the spin and charge sectors, and, as a result, the Chern number of the system is characterized by a hybridization gap in the state of the Kondo lattice at half-filling. The gapless edge states form a surface sub-band of the Fermi surface $\varepsilon_F = 0$ in the insulator phase. The total energy of the system remains the same, it does not depend on the doping of the system, a static $\mathbb{Z}_2$ gauge field “works” as a reservoir for doped particles. In contrast to a traditional insulator phase, the Fermi surface is occupied and an insulator gap is effectively twice as small.

**Conclusions.** – In summary, we have considered the implication of the adiabatic connection between the spin and the fermion subsystem defined on a honeycomb Kondo lattice. There exist two possibilities of realization of the Kondo insulator state, both cases have been considered. We have calculated a hybridization gap in the framework of the model proposed (up to now the mechanism of forming of the hybridization gap in the state of the Kondo insulator has been unknown). The spinless fermions are localized at the lattice sites due to the contact interaction with local moments, this phenomenon is analogous to the Kondo screening in real space (on lattice sites). The itinerant states of spinless fermions hybridize with spin excitations, and, as a result, the gap opens at the half-filling. The gapless edge states form a surface sub-band of chiral Majorana fermions. It is shown that hybridization within a topological Kondo insulator can lead to changing a fermionic topological insulator into a spin one in the sense of low-energy edge excitations.

In the spin-wave approach, the spin excitations are bosons, they are not hybridized with fermions. The ground state of the Kondo lattice at half-filling can be explained by a hybridization gap that arises from a hybridization of itinerant electrons and local moments. In this letter we have firstly proposed the mechanism of hybridization between local spins and itinerant spinless fermions in the framework of the proposed exactly solvable model.

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