We analyze a 2D spin-pseudospin model, where the pseudospins represents the charge degrees of freedom. The model is known to undergo a phase transition with the simultaneous appearance of the long-range charge order and the spin gap. We show how the gap vs critical temperature ratio (also called the BCS ratio) gets renormalized from the classical non-interacting value. This value is also universal in the sense that it does not depend on the microscopic parameters of the model, and must be the same for various types of the Peierls-like transitions where the spin gap is accompanied by the structural, orbital or charge order.

- **Introduction.** – There is a large number of materials which demonstrate phase transitions into states with a spin gap accompanied by some types of the structural, charge or orbital order. The most canonical example is the spin-Peierls transition [1, 2]. The interplay of charge, spin and orbital degrees of freedom is known to produce some exotic phases in transition metal oxides [3]. The dimerized Peierls states driven by the superstructures of the orbital order are reported in some spinels [3]. Our main motivation comes from the recent work on the spin-SAF transition in the quarter-filled ladder compound NaV$_2$O$_5$ [6–10], where the Super-Anti-Ferroelectric (SAF) long-range charge order occurs together with the spin gap. Several other layered vanadate compounds demonstrate transitions when the spin gaps occur simultaneously with charge ordering. In particular, the spin-SAF transition was recently reported in Zn(pyz)V$_4$O$_{10}$ [11].

If, in all seemingly different Peierls-like states the spin gap is induced by the dimerization due to structural, orbital or charge long-range order, then there should be some universal parameters unifying all such transitions. A good candidate is the BCS ratio we calculate here for the case of the spin-SAF transition. It does not depend on the model microscopic parameters and matches the value found earlier for the spin-Peierls transition.

- **Spin-Pseudospin Model and Analysis.** – We analyze here a spin-pseudospin model which consists of the Ising pseudospins $T$ coupled to the Heisenberg spins $S$ which reside on the same sites of a square lattice. The pseudospin sector is given by the Ising Model in a Transverse Field (IMTF). An elementary plaquette and the couplings in this model are shown in Fig. 1. The Hamiltonian of this IMTF reads:

$$H_{\text{IMTF}} = \frac{1}{2} \sum_{nn,nnn} J^\#_{xk} T^z_{k} - \Omega \sum_k T^z_k .$$

(1)

The spin sector is given by the Heisenberg chains parallel to the $J_1$ diagonals $H_S = J \sum_{m,n} S_{mn} S_{m,n+1}$. The spin-pseudospin coupling is:

$$H_{ST} = \frac{1}{2} \varepsilon \sum_{m,n} S_{mn} S_{m,n+1} T^x_{m+1,n+1} - T^x_{m-1,n} ,$$

(2)

with the total Hamiltonian of the model:

$$H = H_{\text{IMTF}} + H_S + H_{ST} .$$

(3)

The spin and pseudospin operators satisfy the standard $SU(2)$ algebra, while $S$ and $T$ commute.

The spin-pseudospin model (3) and some of its modifications were proposed and analyzed in the earlier related work [3, 10] in the context of the quarter-filled ladder compound NaV$_2$O$_5$, where the pseudospins correspond to the charge degrees of freedom. For the physically interesting couplings [10], the classical Ising model ($\Omega = 0$) orders into the 4-fold degenerate Super-Anti-Ferromagnetic (SAF) phase [12] shown in Fig. 1.
FIG. 1: Couplings on an elementary plaquette of the 2D nn and nnn Ising model (left) and an example of the 4-fold degenerate SAF order (right). The SAF is also called columnar or stripe order in some recent literature. The degeneracy of the SAF state is due to the $\mathbb{Z}_2 \otimes \mathbb{Z}_2$ symmetry with respect to the spins of each of the sublattices (labeled by circles or squares) being flipped. The lattice vectors are parameterized by the integers $(m, n)$ in the skewed basis $r = me_1 + ne_2$.

The SAF pattern appears in various contexts, and it is also called columnar or stripe order in some more recent literature. That is what we called the spin-SAF transition \cite{7–10}. Note that the spin gap is due to the frozen phonon displacements at the spin-Peierls transition, while the charge plays the role of phonons at the spin-SAF transition.

The molecular-field approximation is applied for the pseudospins \cite{7}, while the spin sector is treated via minimization of the exact free energy of the dimerized Heisenberg $XXX$-chain

$$H_{xxx} = \sum_n J(1 + (-1)^n)S_nS_{n+1}.$$  \hfill (4)

The specific free energy of the spin chain $f_s(T, \delta)$ is an analytic function at $T \neq 0$ and can be expanded over $\delta$ as $f_s(T, \delta) = f_s(T, 0) - \frac{1}{2} \eta(T, 0) \delta^2 + \mathcal{O}(\delta^3)$, where $\eta(T, 0)$ is called the static dimerization susceptibility.

- **Spin-SAF phase transition.** $XY$ Spin Chain: Free Fermions. – It is straightforward to obtain in a closed form the specific free energy of the $XY$ spin chain mapped onto the spinless non-interacting Jordan-Wigner fermions. To leading order \cite{7}

$$\eta_{XY}(T, 0) = \frac{1}{\pi} \ln \frac{CJ}{T} + \mathcal{O}\left(\frac{T^2}{J^2}\right),$$

where $C \equiv \frac{4}{\pi e \gamma}$, $\gamma = 0.5772...$ is Euler’s constant. In the region $J < J_c$ (where $J_c = 2\Omega$ is the mean-field value of the QCP of the IMTF \cite{11} \cite{10}), the critical temperature is given by the BCS-type solution

$$T_c \approx C J \exp\left[-\frac{\pi J}{\varepsilon^2} (J_c - J)\right].$$

The ground-state dimerization is

$$\delta \approx \frac{4}{e} \exp\left[-\frac{\pi J}{\varepsilon^2} (J_c - J)\right], \quad T = 0.$$  \hfill (7)

In the case of free fermions the spin gap depends linearly on dimerization, $\Delta_{XY} = J\delta$. So the ratio of the zero-temperature spin gap ($\Delta_0$) and the critical temperature (a.k.a the BCS ratio) in the regime $J_c < J$ is

$$\frac{\Delta_{XY}}{T_c} = \frac{4}{eC} = \frac{\pi}{e\gamma} = 1.76...,$$

which coincides exactly with the classical result for the superconducting gap in the BCS theory \cite{14}.

- **Spin-SAF phase transition.** $XXX$ Spin Chain: Interacting Fermions – sine-Gordon Model. – The Heisenberg spin chain can be mapped onto the model of interacting Jordan-Wigner spinless fermions,
the low-energy sector of the fermionic Hamiltonian in its turn can be bosonized [13]. Neglecting the marginal term, the dimerized spin chain maps onto the sine-Gordon model [13]

\[ v^{-1}H_{SG} = \frac{1}{2} \int dx (\Pi^2 + (\partial_x \phi)^2) + 2\mu \int dx \cos \sqrt{2\pi} \phi, \]  

(9)

where \( v = \frac{\pi}{2} J \) is the bosonic velocity and \( \mu = \frac{A_0}{\pi} \delta \). The relevant perturbation of the free bosonic part of the Hamiltonian (9) comes from the spin dimerization term \((-1)^n S_n S_{n+1} \sim A_\epsilon \cos \sqrt{2\pi} \phi \). The amplitude \( A_\epsilon \) is not known exactly yet, but according to the approximate calculations of Orignac [16]

\[ A_\epsilon = \frac{3}{\pi^2} (\frac{\pi}{2})^{\frac{1}{4}} \]  

(10)

Using the sine-Gordon model (9) to approximate the low-energy sector of the dimerized Heisenberg chain (4), the free energy of the latter reads to leading order [13, 17]

\[ f_s(T, \delta) = -J t_o - \frac{1}{3} J^2 - \frac{1}{2} \frac{J^2 a_o}{T} \delta^2, \]  

where \( a_o = \frac{1}{4} (\Gamma(1/4)/\Gamma(3/4))^2 A_\epsilon^2 \equiv \partial_1 A_\epsilon^2 \),

(11)

and \( t_o \equiv \ln 2 - \frac{1}{4} = 0.4431\ldots \). Then the dimerization susceptibility to lowest order

\[ \eta(T, 0) = \frac{a_o J}{T}. \]  

(12)

This function was first calculated by Cross and Fisher [2] for their spin-Peierls transition theory. The amplitude \( A_\epsilon [10] \) suggested by Orignac [16] gives \( a_o = 0.253418 \), very close to the original bosonization result \( a^{CF}_o \approx 0.26 \) [2].

The interactions of the Jordan-Wigner spinless fermions of the XXX chain modify considerably the critical properties of the Ising-XXX model [3]. The inverse dependence \( \eta \propto T^{-1} \) results in the power-law dependence of \( T_c \) on couplings:

\[ T_c = \partial_1 A_\epsilon^2 \frac{\delta^2}{\mathcal{J}_c - \mathcal{J}}, \]  

\[ \mathcal{J} < \mathcal{J}_c. \]  

(13)

The phase diagram of the Ising-XXX model is shown in Fig. 2.

FIG. 2: Phase diagram of the coupled Ising-XXX model. Axes are not in scale. The solid red line shows the critical temperature \( T_c \) separating the disordered and SAF phases of the decoupled IMTF. Its QCP corresponds to \( \mathcal{J}_c = 2\Omega \) in the mean-field approximation. (\( \mathcal{J} = J_1 + J_2 \)). The dashed blue line shows \( T_c \) separating the disordered + spin gapless phase from the spin-SAF phase of the coupled Ising-XXX model.

From the ground-state specific energy of the sine-Gordon model [15, 18]

\[ f_{SG}(0, \mu) = -v^2 M^2 \tan \frac{\pi}{6}, \]  

where \( M = \frac{2}{\sqrt{\pi}} \left( \frac{\Gamma(3/4)}{\Gamma(1/4)} \right)^{2/3} \frac{\Gamma(1/6)}{\Gamma(2/3)} \)

(14)
(M is the dimensionless soliton mass) we get the ground-state energy of the Heisenberg chain (4):

$$f_s(0, \Delta_o) = -Jt_o - \frac{1}{2\pi\sqrt{3}} \frac{\Delta_o^2}{J}, \quad (15)$$

where the zero-temperature spin gap $\Delta_o = \frac{\pi}{2}JM$ is related to the dimerization as follows:

$$\Delta_o = J \sqrt{\pi} \left( \frac{\Gamma(3/4)}{\Gamma(1/4)} \right)^{2/3} \frac{\Gamma(1/6)}{\Gamma(2/3)} A^2 \delta^{2/3}. \quad (16)$$

The ground-state spin gap:

$$\Delta_o = \vartheta_2 A^2 \frac{\varepsilon^2}{J_c - J}, \quad \text{where } \vartheta_2 \equiv \frac{2}{3} \sqrt{\frac{\pi}{3}} \left( \frac{\Gamma(3/4)}{\Gamma(1/4)} \right)^2 \left( \frac{\Gamma(1/6)}{\Gamma(2/3)} \right)^3 \quad (17)$$

Combining Eqs. (13,17) we obtain the BCS ratio:

$$\frac{\Delta_o}{J_c} = \frac{\vartheta_2}{\vartheta_1} = 6\sqrt{3} \left( \frac{\Gamma(1/3)}{\Gamma(1/4)} \right)^9 = 2.47... \quad (18)$$

The same BCS ratio for the spin-Peierls transition was first obtained by Orignac and Chitra [17]. We would like to stress that the above result is exact for the IMTF coupled to the sine-Gordon model, i.e., when the marginal terms in the Heisenberg spin Hamiltonian are neglected. Similar to the non-interacting result [8], the ratio [18] does not depend on the microscopic parameters of the model, and even the dimerization amplitude $A_c$ cancels. In this sense we interpret this as a universal result. The interactions renormalize the BCS ratio away from the free fermionic value of 1.76.

**Conclusions.** – The BCS ratio in the interacting Ising-XXX model is calculated. Similar to the classical free-fermionic case, this value is also universal in the sense that is does not depend on the microscopic parameters of the model. We conjecture that it must be the same for various types of the Peierls-like transitions where the spin gap is accompanied by the structural, orbital or charge order. An extension of these results taking into account marginal terms of the spin chain Hamiltonian is warranted.

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