Quantum phase transitions in a strongly entangled spin-orbital chain: A field-theoretical approach

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Quantum phase transitions in a strongly entangled spin-orbital chain: A field-theoretical approach

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Motivated by recent experiments on quasi-1D vanadium oxides, we study quantum phase transitions in a one-dimensional spin-orbital model describing a Haldane chain and a classical Ising chain locally coupled by the relativistic spin-orbit interaction. By employing a field-theoretical approach, we analyze the topology of the ground-state phase diagram and identify the nature of the phase transitions. In the strong coupling limit, a long-range Néel order of entangled spin and orbital angular momentum appears in the ground state. We find that, depending on the relative scales of the spin and orbital gaps, the linear chain follows two distinct routes to reach the Néel state. First, when the orbital exchange is the dominating energy scale, a two-stage ordering takes place in which the magnetic transition is followed by melting of the orbital Ising order; both transitions belong to the two-dimensional Ising universality class. In the opposite limit, the low-energy orbital modes undergo a continuous reordering transition which represents a line of Gaussian critical points. On this line the orbital degrees of freedom form a Tomonaga-Luttinger liquid. We argue that the emergence of the Gaussian criticality results from merging of the two Ising transitions in the strong hybridization region where the characteristic spin and orbital energy scales become comparable. Finally, we show that, due to the spin-orbit coupling, an external magnetic field acting on the spins can induce an orbital Ising transition.

PACS numbers:

I. INTRODUCTION

Over the past decades, one-dimensional spin-orbital models have been a subject of intensive theoretical studies. The interest is to a large extent motivated by experimental discovery of unusual magnetic properties in various quasi-one-dimensional Mott insulators.[1,2] The inter-dependence of spin and orbital degrees of freedom is usually described by the so-called Kugel-Khomskii Hamiltonian in which the effective spin exchange constant depends on the orbital configuration and vice versa.[3,4] Another mechanism of coupling spin and orbital degrees of freedom is the on-site relativistic spin-orbit (SO) interaction $\lambda\,\mathbf{L}\cdot\mathbf{S}$, where $\mathbf{L}$ is the orbital angular momentum and λ is the coupling constant. In compounds with quenched orbital degrees of freedom, the presence of the SO term usually leads to the single-ion spin anisotropy DS_z^2 where $D \sim \lambda^2/\Delta$ and Δ denotes the energy scale of the crystal field which lifts the degenerate orbital states.

For systems with residual orbital degeneracy, on the other hand, the effect of the SO term is much less explored compared with the Kugel-Khomskii-type coupling. Due to the directional dependence of the orbital wave functions, the SU(2) symmetry of the Heisenberg spin exchange is expected to be broken in the presence of the SO interaction. The resultant spin anisotropy is likely to induce a long-range magnetic order in the spin sector. A more intriguing question is what happens to the orbital sector. To answer this question, one needs to consider the details of the interplay between the orbital exchange and the SO coupling. Here we consider the simplest case of a two-fold orbital degeneracy per site. Specifically, the two degenerate states could be the d_{yz} and d_{zx} orbitals in a tetragonal crystal field observed in several transition-metal compounds. We introduce pseudospin-1/2 operators τ^a $(a = x, y, z)$ to describe the doublet orbital degrees of freedom assuming that $\tau^z = \pm 1$ correspond to the states $|yz\rangle$ and $i|zx\rangle$, respectively. Alternatively, one can also realize the double orbital degeneracy in the Mott-insulating phase of a 1D fermionic optical lattice where the eigenvectors of τ^z refers to p_x and p_y orbitals in an anisotropic potential.[5,6] Restricted to this doublet space, the orbital angular momentum operator $\mathbf{L} = (0, 0, \tau^x)$. This can be easily seen by noting that the eigenstates of τ^x carry an angular momentum $\langle L^z\rangle = \pm 1$.

The exchange interaction between localized orbital degrees of freedom is characterized by its highly directional dependence: the interaction energy only depends on whether the relevant orbital is occupied for bonds of a given orientation. This is particularly true for interactions dominated by direct exchange mechanism. Denoting the relevant orbital projectors on a given bond as $P = (1 + \tau^\beta)/2$, where $\tau^\beta/2$ is an appropriate pseudospin-1/2 operator (τ^β being a Pauli matrix), the orbital interaction is thus described by an Ising-type term $\tau_i^\beta \tau_j^\beta$. The well studied orbital compass model and Kitaev model both belong to this category.[7,8] The quantum nature of these models comes from the fact that different operators τ^β, which do not commute with each other, are used for bonds of different types. To avoid unnecessary complications coming from the details of orbital interactions, we assume that there is only one type of bond in our 1D system and the orbital interaction is thus governed by a classical Ising Hamiltonian.

We incorporate these features into the following toy model of spin-orbital chain ($J_s, J_\tau > 0$):

$$\begin{aligned} H &= H_S + H_\tau + H_{S\tau} \\ &= J_S \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + J_\tau \sum_n \tau^z_n \tau^z_{n+1} + \lambda \sum_n \tau^x_n S^z_n. \end{aligned} \tag{1}$$

Motivated by the recent experimental characterizations of quasi-1D vanadium oxides,[14–19] here we focus on the case of quantum spin with length $S = 1$. The above model thus describes a Haldane chain locally coupled to a classical Ising chain by the SO interaction $H_{S\tau}$. The role of the λ-term is two-fold: firstly it introduces anisotropy to the spin-1 subsystem, and secondly it endows quantum dynamics to the otherwise classical Ising chain.

Before turning to a detailed study of the phase diagram of model (1), we first discuss its connections to real compounds. As mentioned above, the interest in the toy model is partly motivated by the recent experimental progress on vanadium oxides which include spinel ZnV_2O_4[14–17] and quasi-1D CaV_2O_4.[18,19] In both types of vanadates, the two d electrons of V^{3+} ions have a spin $S = 1$ in accordance with Hund's rule. In the low-temperature phase of both vanadates, the vanadium site embedded in a flattened VO_6 octahedron has a tetragonal symmetry. This tetragonal crystal field splits the degenerate t_{2g} triplet into a singlet and a doublet. As one of the two d electrons occupies the lower-energy d_{xy} state, a double orbital degeneracy arises as the second electron could occupy either d_{zx} or d_{yz} orbitals. The fact that the d_{xy} orbital is occupied everywhere also contributes to the formation of weakly coupled quasi-1D spin-1 chains in these compounds.[20] On the other hand, the details of the orbital exchange depends on the geometry of the lattice and in the case of vanadium spinel the orbital interaction is of three-dimensional nature. The Ising orbital Hamiltonian in Eq. (1) thus should be regarded as an effective interaction in the mean-field sense. Nonetheless, the toy model provides a first step towards understanding the essential physics introduced by the SO coupling. Moreover, many conclusions of this paper can be applied to the case of quasi-1D compound CaV_2O_4 where the vanadium ions form a zigzag chain.

It is instructive to first establish regions of stable massive phases. In the decoupling limit, $\lambda \to 0$, our model describes two gapped systems: a quantum spin-1 Heisenberg chain and a classical orbital Ising chain. The ground state of the spin sector is a disordered quantum spin liquid with a finite spectral gap[21] Δ_S, whereas the orbital ground state is characterized by a classical Néel order along the chain: $\langle \tau^z_n \rangle = (-1)^n \eta^z$. Quantum effects in the orbital sector induced by the SO coupling play a minor role. Obviously, just because of being gapped, both the spin-liquid phase and the orbital ordered state are stable as long as λ remains small. Consider now the opposite limit, $\lambda \gg J_S, J_\tau$. In the zeroth order approximation, the model is dominated by the single-ion term $H_{S\tau}$ whose doubly degenerate eigenstates $|\pm\rangle = |S^z = \pm 1\rangle \otimes |\tau^x = \pm 1\rangle$ represent locally entangled spin and orbital degrees of freedom. Switching on small J_S and J_τ leads to a staggered ordering of the $|+\rangle$ and $|-\rangle$ states along the chain. Physically, the large-λ ground state can be viewed as a simultaneous Néel ordering of spin and orbital angular momentum characterized by order parameters ζ and η^x such that $\langle S^z_n \rangle = (-1)^n \zeta$ and $\langle L^z_n \rangle = \langle \tau^x_n \rangle = (-1)^n \eta^x$. The Ising order parameter η^z vanishes identically in this phase.

These observations naturally lead to the following questions. How is the magnetically ordered Néel state at large λ connected to the disordered Haldane phase as $\lambda \to 0$? What is the scenario for the orbital reorientation transition $\eta^z \to \eta^x$, which is of essentially quantum nature ? In this paper we employ the field-theoretical approach to address these questions. We first note that the one-dimensional model (1) is not exactly integrable. As a consequence, the regime of strong hybridization of the spin and orbital excitations, which is the case when J_τ, J_S and λ are all of the same order, stays beyond the reach of approximate analytical methods. We thus will be mainly dealing with limiting cases $J_\tau \gg J_S$ and $J_\tau \ll J_S$, in which one can integrate out the "fast" variables to obtain an effective action for the "slow" modes. Following this approach, we establish the topology and main features of the ground-state phase diagram in the accessible parts of the parameter space of the model. We were able to unambiguously identify the universality classes of quantum criticalities separating different massive phases. Using plausible arguments we comment on some features of the model in the regime of strong spin-orbital hybridization.

We demonstrate that the aforementioned reorientation transition $\eta^z \to \eta^x$ can be realized in one of two possible ways. In the limit of large J_τ, we find a sequence of two quantum Ising transitions and an intermediate massive phase, sandwiched between these critical lines, in which both η^z and η^x are nonzero. This is consistent with the recent findings[22] based on DMRG calculations and some analytical estimations. In the opposite limit, when the Haldane gap Δ_S is the largest energy scale, integrating out the spin excitations yields an effective lowest-energy action for the orbital degrees of freedom, which shows that the $\eta^z \to \eta^x$ crossover takes place as a single Gaussian quantum criticality. At this critical point, the orbital degrees of freedom display an extremely quantum behaviour: they are gapless and form a Tomonaga-Luttinger liquid. This is the main result of this paper. We bring about arguments suggesting that the emergence of the Gaussian critical line is the result of merging of the two Ising criticalities in the region of strong spin-orbital hybridization.

Any field-theoretical treatment of the model (1) must be based on a properly chosen contiuum description of the spin-1 antiferromagnetic Heisenberg chain. Its properties have been thoroughly studied, both analytically and numerically (see for a recent review Ref. 23). In what follows, the spin sector of the model (1) will be treated within the O(3)-symmetric Majorana field theory, proposed by Tsvelik:[24]

$$\mathcal{H}_{\rm M} = \sum_{a=1,2,3}\left[\frac{{\rm i}v}{2}\left(\xi^a_L\partial_x\xi^a_L - \xi^a_R\partial_x\xi^a_R\right) - {\rm i}m\xi^a_R\xi^a_L\right] + \mathcal{H}_{\rm int}. \tag{2}$$

Here $\xi^a_{R,L}(x)$ is a degenerate triplet of real (Majorana) Fermi fields with a mass m, the indices R and L label the chirality of the particles, and

$$\mathcal{H}_{\rm int} = \frac{1}{2}g\sum_a\left(\xi^a_R\xi^a_L\right)^2$$

is a weak four-fermion interaction which can be treated perturbatively. The continuum theory (2) adequately describes the low-energy properties of the generalized spin-1 bilinear-biquadratic chain

$$H_S \to \bar{H}_S = J_S\sum_n\left[\mathbf{S}_n\cdot\mathbf{S}_{n+1} - \beta\left(\mathbf{S}_n\cdot\mathbf{S}_{n+1}\right)^2\right]. \tag{3}$$

in the vicinity of the critical point $\beta = 1$.[25] This quantum criticality belongs to the universality class of the $\mathrm{SU}(2)_2$ Wess-Zumino-Novikov-Witten (WZNW) model with central charge $c = 3/2$.

At small deviations from criticality the Majorana mass $m \sim J_S|\beta-1|$ determines the magnitude of the triplet gap, $\Delta_S = |m| \ll J_S$. The theory of a massive triplet of Majorana fermions is equivalent to a system of three degenerate noncritical 2D Ising models, with $m \sim (T-T_c)/T_c$. This is one of the most appealing features of the theory because the most strongly fluctuating physical fields of the $S = 1$ chain, namely the staggered magnetization and dimerization operators, have a simple local representation in terms of the Ising order and disorder parameters.[24,26,27] It is this fact that greatly simplifies the analysis of the spin-orbital model (1). While the correspondence between the models (2) and (3) is well justified at $|\beta-1| \ll 1$, it is believed that the Majorana model (2) captures generic properties of the Haldane spin-liquid phase of the spin-1 chain, even though at large deviations from criticality ($|\beta-1| \sim 1,\ \Delta_S \sim J_s$) all parameters of the model should be treated as phenomenological.

The remainder of the paper is organized as follows. We start our discussion with Sec. II which contains a brief summary of known facts about the Majorana model[24] that will be used in the rest of the paper. In Sec. III we consider the limit $J_\tau/\Delta_S \gg 1$ and by integrating out the 'fast' orbital modes, show that on increasing the SO coupling λ the system undergoes a sequence of two consecutive quantum Ising transitions in the spin and orbital sectors, respectively. In section IV we analyze the opposite limiting case, $J_\tau/\Delta_S \ll 1$, and, by integrating over the 'fast' spin modes, show that there exists a single Gaussian transition in the orbital sector accompanied by a Neel ordering of the spins. We then conjecture on the topology of the ground-state phase diagram of the model. In Sec. V we show that spin-orbital hybridization effects near the orbital Gaussian transition lead to the appearance of a non-zero spectral weight well below the Haldane gap which can be detected by inelastic neutron scattering experiments and NMR measurements. In Sec. VI we comment on the role of an external magnetic field. We show that, through the SO interaction, a sufficiently strong magnetic field affects the orbital degrees of freedom and can lead to a quantum Ising transition in the orbital sector. Sec. VII contains a summary of the obtained results and conclusions. The paper has two appendices containing certain technical details.

II. SOME FACTS ABOUT MAJORANA THEORY OF SPIN-1 CHAIN

In this Section, we provide some details about the O(3)-symmetric Majorana field theory,[24] Eq. (2), which represents the continuum limit of the biquadratic spin-1 model (3) at $|\beta-1| \ll 1$.

In the continuum description, the local spin density of the spin model (3) has contributions from the low-energy modes centered in momentum space at $q = 0$ and $q = \pi$:

$$\mathbf{S}(x) = \mathbf{I}_R(x) + \mathbf{I}_L(x) + (-1)^{x/a_0}\mathbf{N}(x) \tag{4}$$

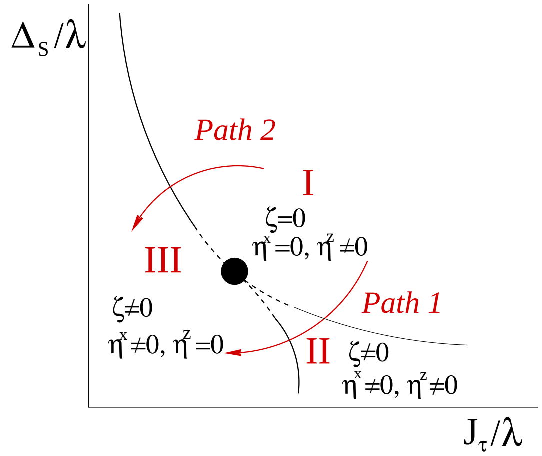

FIG. 1: Schematic phase diagram of the model on the $(x_S,\, x_\tau)$-plane, where $x_S = \Delta_S/\lambda$ and $x_\tau = J_\tau/\lambda$.

The smooth part of the local magnetization, $\mathbf{I} = \mathbf{I}_R + \mathbf{I}_L$, is a sum of the level-2 chiral vector currents. The $SU(2)_2$ Kac-Moody algebra of these currents is faithfully reproduced in terms of a triplet of massless Majorana fields[28] $\boldsymbol{\xi} = (\xi^1, \xi^2, \xi^3)$:

$$\mathbf{I}_\nu = -\frac{i}{2}\left(\boldsymbol{\xi}_\nu \times \boldsymbol{\xi}_\nu\right), \quad (\nu = R, L) \tag{5}$$

This fact is not surprising because, as already mentioned, the central charge of the $SU(2)_2$ WZNW theory is $c = 3/2$, whereas that of the theory of a massless Majorana fermion (equivalently, critical 2D Ising model) is $c = 1/2$. At small deviations from criticality ($|\beta - 1| \ll 1$) the fermions acquire a mass. Strongly fluctuating fields of the spin-1 chain, the staggered magnetization $\mathbf{N}(x)$ and dimerization operator $\epsilon(x) = (-1)^n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$, are nonlocal in terms of the Majorana fields but admit a simple representation in terms of the order, σ, and disorder, μ, operators of the related noncritical Ising models:

$$\begin{aligned} \mathbf{N} &\sim (1/\alpha)\left(\sigma_1\mu_2\mu_3,\ \mu_1\sigma_2\mu_3,\ \mu_1\mu_2\sigma_3\right), \\ \epsilon &\sim (1/\alpha)\,\sigma_1\sigma_2\sigma_3, \end{aligned} \tag{6}$$

where $\alpha \sim a_0$ is a short-distance cutoff of the continuum theory. These expressions together with their duals (i.e. their counterparts obtained by the duality transformation in all Ising copies, $\sigma_a \leftrightarrow \mu_a$) determine the vector and scalar parts of the WZNW 2×2 matrix field $\hat{g}$ which is a primary scalar field with scaling dimension $3/8$. It has been demonstrated in Ref. 28 that using the representation (6) and the short-distance operator product expansions for the Ising fields, one correctly reproduces all fusion rules of the $SU(2)_2$ WZNW model. An equivalent way to make sure that this is indeed the case is to consider the four-Majorana representation of the weakly coupled spin-1/2 Heisenberg ladder[26,27] and take the limit of a infinite singlet Majorana mass to map the low-energy sector of the model on the O(3) theory (2).

In the spin-liquid phase of the spin chain (3), which is the case $\beta < 1$, the Majorana mass m is positive, implying that the degenerate triplet of 2D Ising models is in a disordered phase: $\langle\sigma_a\rangle = 0$, $\langle\mu_a\rangle \neq 0$ $(a = 1, 2, 3)$. In particular, this implies that the O(3) symmetry remains unbroken, $\langle\mathbf{N}\rangle = 0$, and the ground state of the system is not spontaneously dimerized, $\langle\epsilon\rangle = 0$.

The representation (6) proves to be very useful for calculating the dynamical spin correlation functions because the asymptotics of the Ising correlators $\langle\sigma(x,\tau)\sigma(0,0)\rangle$ and $\langle\mu(x,\tau)\mu(0,0)\rangle$ are well known both at criticality and in a noncritical regime. In the disordered phase ($m > 0$), the leading asymptotics of the Ising correlators are:

$$\begin{aligned} \langle\mu(\mathbf{r})\mu(\mathbf{0})\rangle &\sim (a/\xi_S)^{1/4}\left[1 + O(e^{-2r/\xi_S})\right], \\ \langle\sigma(\mathbf{r})\sigma(\mathbf{0})\rangle &\sim (a/\xi_S)^{1/4}\sqrt{\xi_S/r}\; e^{-r/\xi_S} \end{aligned} \tag{7}$$

where $\xi_S = v/m$ is the correlation length, and $r = \sqrt{x^2 + v^2\tau^2}$. (By duality, in the ordered phase ($m < 0$) the asymptotics of the correlators in (7) must be interchanged.) Correspondingly, the dynamical correlation function

$$\langle\mathbf{N}(\mathbf{r})\mathbf{N}(\mathbf{0})\rangle \sim (a/\xi_S)^{3/4}\sqrt{\xi_S/r}\; e^{-r/\xi_S}. \tag{8}$$

Its Fourier transform at $q \sim \pi$ and small ω describes a coherent excitation – a triplet magnon with the mass gap m:

$$\Im m\ \chi(q,\omega) \sim \frac{m}{|\omega|}\delta\left(\omega - \sqrt{(q-\pi)^2 v^2 + m^2}\right). \tag{9}$$

Since the single-ion anisotropy $H_{\rm anis} = D\sum_n (S_n^z)^2$ lowers the original O(3) symmetry down to O(2) $\times$ Z$_2$, one expects[24] that in the continuum theory it will induce anisotropy in the Majorana masses

$$m_1 = m_2 \neq m_3,$$

as well as in the coupling constants parametrizing the four-fermion interaction:

$$\mathcal{H}_{\rm int} \to \frac{1}{2}\sum_{a\neq b} g_{ab}\left(\xi_R^a\xi_L^a\right)\left(\xi_R^b\xi_L^b\right), \quad g_{13} = g_{23} \neq g_{12}\ .$$

This can be checked by using the correspondence (4) and short-distance operator product expansions (OPE) for the physical fields. There will also appear anisotropy in the velocities, $v_1 = v_2 \neq v_3$, but we will systematically neglect this effect. Thus, we have $H_{\rm anis} = \int {\rm d}x\ \mathcal{H}_{\rm anis}$, with

$$\mathcal{H}_{\rm anis} = D\alpha \int {\rm d}x\left[I^3(x)I^3(x+\alpha) + N^3(x)N^3(x+\alpha)\right], \tag{10}$$

where $\alpha \sim a$ is a short-distance cutoff of the continuum theory. Using (5) and keeping only the Lorentz invariant terms (i.e. neglecting renormalization of the velocities) we can replace $(I^3)^2$ by $2I_R^3 I_L^3$. To treat the second term in the r.h.s. of (10), we need OPEs for the products of Ising operators:[29]

$$\begin{aligned}&\sigma(z,\bar z)\sigma(w,\bar w)\\ &= \frac{1}{\sqrt{2}}\left(\frac{\alpha}{|z-w|}\right)^{1/4}\left[1 - \pi|z-w|\varepsilon(w,\bar w)\right],\end{aligned} \tag{11}$$

$$\begin{aligned}&\mu(z,\bar z)\mu(w,\bar w)\\ &= \frac{1}{\sqrt{2}}\left(\frac{\alpha}{|z-w|}\right)^{1/4}\left[1 + \pi|z-w|\varepsilon(w,\bar w)\right].\end{aligned} \tag{12}$$

Here $\varepsilon = i\xi_R\xi_L$ is the energy density (mass bilinear) of the Ising model, $z = v\tau + {\rm i}x$ and $w = v\tau' + {\rm i}x'$ are two-dimensional complex coordinates, $\bar z$ and $\bar w$ are their conjugates. From the above OPEs it follows that

$$\begin{aligned}N^3(x)N^3(x+\alpha) &= {\rm i}(\pi/\alpha)\left(\xi_R^1\xi_L^1 + \xi_R^2\xi_L^2 - \xi_R^3\xi_L^3\right)\\ &-(\pi^2 C)[(\xi_R^1\xi_L^1)(\xi_R^2\xi_L^2) - (\xi_R^1\xi_L^1)(\xi_R^3\xi_L^3) - (\xi_R^2\xi_L^2)(\xi_R^3\xi_L^3)],\end{aligned}$$

where $C \sim 1$ is a nonuniversal constant. As a result,

$$\mathcal{H}_{\rm anis} = -{\rm i}\sum_{a=1,2,3}\delta m_a\ \xi_R^a\xi_L^a + \frac{1}{2}\sum_{a\neq b}\delta g_{ij}\left(\xi_R^a\xi_L^a\right)\left(\xi_R^b\xi_L^b\right), \tag{13}$$

where

$$\delta m_1 = \delta m_2 = -\delta m_3 = -(\pi C)D \tag{14}$$

are corrections to the single-fermion masses, and $\delta g_{12} = (2-\pi^2 C)D\alpha$, $\delta g_{13} = \delta g_{23} = \pi^2 C D\alpha$ are coupling constants of the induced interaction between the fermions. Smallness of the Majorana masses ($|m|\alpha/v \ll 1$) implies that the additional mass renormalizations caused by the interaction in (13) are relatively small, $m(D\alpha/v)\ln(v/|m|\alpha) \ll D$, so that the main effect of the single-ion anisotropy is the additive renormalization of the fermionic masses, $m_a = m + \delta m_a$, with δm_a given by Eq.(14).

The cases $D > 0$ and $D < 0$ correspond to an easy-plane and easy-axis anisotropy, respectively. The spin anisotropy (18) induced by the spin-orbit coupling is of the easy-axis type. At $D < 0$ the singlet Majorana fermion, ξ^3, is the lightest, $m_3 < m_1 = m_2$. Increasing anisotropy drives the system towards an Ising criticality at $D = -D^*$, where $m_3 = 0$. At $D < -D^*$ the system occurs in a new phase where the Ising doublet remains disordered while the singlet Ising system becomes ordered. It then immediately follows from the representation (6) that the new phase is characterized by a Néel long-range order with $\langle N^3\rangle \neq 0$. Transverse spin fluctuations, as well as fluctuations of dimerization, are incoherent in this phase.

III. TWO ISING TRANSITIONS IN THE $\Delta_S \ll J_\tau$ LIMIT

Now we turn to our model (1). Let us consider the case when, in the absence of spin-orbit coupling, the orbital gap is the largest: $J_\tau \gg J_s$. The orbital pseudospins then represent the 'fast' subsystem and can be integrated out. Assuming that $\lambda \ll J_\tau$, we treat the spin-orbit coupling perturbatively. In this case, the zero order Hamiltonian $H_0 = H_S + H_\tau$ describes decoupled spin and orbital systems, while the spin-orbit interaction $H_{S\tau}$ denotes perturbation. Defining the interaction representation for all operators according to $A(\tau) = e^{\tau H_0} A e^{-\tau H_0}$ (here τ denotes imaginary time), the interaction term in the Euclidian action is given by

$$S_{S\tau} = \lambda \sum_n \int \mathrm{d}\tau \; \tau_n^x(\tau) S_n^z(\tau). \tag{15}$$

The first nonvanishing correction to the effective action in the spin sector is of the second order in λ:

$$\Delta S_s = \frac{-\lambda^2}{2} \sum_{nm} \int \mathrm{d}\tau_1 \mathrm{d}\tau_2 \big\langle \tau_n^x(\tau_1) \tau_m^x(\tau_2) \big\rangle_\tau S_n^z(\tau_1) S_m^z(\tau_2). \tag{16}$$

Averaging in the right-hand side of (16) goes over configurations of the classical Ising chain H_τ. The correlation function $\langle \tau_n^x(\tau_1) \tau_m^x(\tau_2) \rangle_\tau$ is calculated in Appendix A. It is spatially ultralocal (because there are no propagating excitations in the classical Ising model) and rapidly decaying at the characteristic time $\sim 1/J_\tau$, which is much shorter than the spin correlation time $\sim 1/\Delta_0$:

$$\langle \tau_n^x(\tau_1) \tau_m^x(\tau_2) \rangle_\tau = \delta_{nm} \exp\left(-4J_\tau |\tau_1 - \tau_2|\right). \tag{17}$$

Passing to new variables, $\tau = (\tau_1 + \tau_2)/2$ and $\rho = \tau_1 - \tau_2$, and integrating over ρ yields a correction to the effective spin action which has the form of a single-ion spin anisotropy. Thus in the second order in λ, the spin Hamiltonian acquires an additional term

$$H_{\mathrm{ani}} = -\frac{\lambda^2}{4J_\tau} \sum_n \left(S_n^z\right)^2. \tag{18}$$

The anisotropy splits the Majorana triplet into a doublet (ξ^1, ξ^2) and singlet (ξ^3), with masses

$$m_1 = m_2 = m + \frac{\pi C \lambda^2}{4J_\tau}, \quad m_3 = m - \frac{\pi C \lambda^2}{4J_\tau}, \tag{19}$$

where $C \sim 1$ is a nonuniversal positive constant. The anisotropy is of the easy-axis type, so that the singlet mode has a smaller mass gap.

As long as all the masses m_a remain positive, the system maintains the properties of an anisotropic Haldane's spin-liquid. The dynamical spin susceptibilities calculated at small ω and $q \sim \pi$ (see Sec. II),

$$\begin{aligned} \Im m\, \chi^{xx}(q,\omega) &= \Im m\, \chi^{yy}(q,\omega) \\ &\sim \frac{m_1}{|\omega|} \delta\left(\omega - \sqrt{(q-\pi)^2 v^2 + m_1^2}\right), \\ \Im m\, \chi^{zz}(q,\omega) &\sim \frac{m_3}{|\omega|} \delta\left(\omega - \sqrt{(q-\pi)^2 v^2 + m_3^2}\right), \end{aligned} \tag{20}$$

indicate the existence of the $S^z = \pm 1$ and $S^z = 0$ optical magnons with mass gaps m_1 and m_3, respectively. Increasing the spin-orbital coupling leads eventually to an Ising criticality at $\lambda = \lambda_{c1} = 2\sqrt{J_\tau m / \pi C}$, where $m_3 = 0$. At $m_3 < 0$ the system occurs in a long-range ordered Néel phase with staggered magnetization $\langle S_n^z \rangle = (-1)^n \zeta(\lambda)$, in which the Z_2-symmetry of model (18) is spontaneously broken. Using the Ising-model representation (6) of the staggered magnetization of the spin-1 chain, we find that at $0 < \lambda - \lambda_{c1} \ll \lambda_{c1}$ the order parameter $\zeta(\lambda)$ follows a power-law increase:

$$\zeta(\lambda) \sim \left(\frac{\lambda - \lambda_{c1}}{\lambda_{c1}}\right)^{1/8}. \tag{21}$$

The transverse spin fluctuations become incoherent in this phase. The situation here is entirely similar to that in the spontaneously dimerized massive phase of a two-chain spin-1/2 ladder[27,30], where the dimerization kinks make spin fluctuations incoherent. In the present case, the spontaneously broken Z_2 symmetry of the Neel phase leads to the existence of pairs of massive topological kinks contributing to a broad continuum with a threshold at $\omega = m_1 + |m_3|$ (the details of calculation can be found in Ref.27):

$$\Im m\ \chi^{xx}(q,\omega) \sim \frac{1}{\sqrt{m_1|m_3|}} \frac{\theta(\omega^2 - (q-\pi)^2 v^2 - (m_1+|m_3|)^2)}{\sqrt{\omega^2 - (q-\pi)^2 v^2 - (m_1+|m_3|)^2}}. \tag{22}$$

In the Néel phase, the orbital sector acquires quantum dynamics because antiferromagnetic ordering of the spins generates an effective transverse magnetic field which transforms the classical Ising model H_τ to a quantum Ising chain. At $\lambda > \lambda_{c1}$ the spin-orbit term takes the form

$$H_{S\tau} = -h \sum_n (-1)^n \tau_n^x + H'_{S\tau}, \tag{23}$$

where $h = \lambda\zeta(\lambda)$ and $H'_{S\tau} = -\lambda \sum_n \left(S_n^z - \langle S_n^z \rangle\right) \tau_n^x$ accounts for fluctuations. Since both the orbital and spin sectors are gapped, the main effect of this term is a renormalization of the mass gaps and group velocities. The transverse field h gives rise to quantum fluctuations which decrease the classical value of η^z and, at the same time, lead to a staggered ordering of the orbital pseudospins in the transverse direction. Since the orbital sector has a finite susceptibility with respect to a transverse staggered field, in the right vicinity of the critical point η^x follows the same power-law increase as ζ but with a smaller amplitude:

$$\eta^x \sim \left(\frac{h}{J_\tau}\right) \sim \sqrt{\frac{\Delta_S}{J_\tau}} \left(\frac{\lambda - \lambda_{c1}}{\lambda_{c1}}\right)^{1/8}. \tag{24}$$

This result is in a good agreement with previously obtained numerical results for order parameters (See Fig. 4(a) in Ref. 22).

Performing an inhomogeneous π-rotation of the pseudospins around the y-axis, $\tau_n^{x,z} \to (-1)^n \tau_n^{x,z}$, $\tau_n^y \to \tau_n^y$, we find that at $\lambda > \lambda_{c1}$ the effective model in the orbital sector reduces to a ferromagnetic Ising chain in a uniform transverse (pseudo)magnetic field:

$$H_{\tau;\mathrm{eff}} = -J_\tau \sum_n \tau_n^z \tau_{n+1}^z - h \sum_n \tau_n^x. \tag{25}$$

Notice that the restriction $\lambda \ll J_\tau$, which was imposed in the derivation of the effective Hamiltonian in the spin sector, now can be released because the spin sector is assumed to be in the Néel phase.

At $h = J_\tau$, i.e. at $\lambda = \lambda_{c2}$ where λ_{c2} satisfies the equation

$$\lambda_{c2}\ \zeta(\lambda_{c2}) = J_\tau, \tag{26}$$

the model (25) undergoes a 2D Ising transition[27,31] to a massive disordered phase with $\langle \tau_n^z \rangle = 0$. This quantum critical point can be reached when λ is further increased in the region $\lambda > \lambda_{c1}$. It is clear from (26) that λ_{c2} is of the order of or greater than J_τ. It is reasonable to assume that for such values of λ the Néel magnetization is close to its nominal value, $\zeta \sim 1$, implying that $\lambda_{c2} \sim J_\tau$. We see that the two Ising transitions are well separated:

$$\lambda_{c2}/\lambda_{c1} \sim (J_\tau/\Delta_S)^{1/2} \gg 1. \tag{27}$$

Thus, in the limit $J_\tau \gg \Delta_S$, the ground-state phase diagram of the model (1) consists of three gapped phases separated by two Ising criticalities, one in the spin sector ($\lambda = \lambda_{c1}$) and the other in the orbital sector ($\lambda = \lambda_{c2}$). At $0 < \lambda < \lambda_{c1}$ the spin sector represents an anisotropic spin-liquid while in the orbital sector there is a Néel-like ordering of the pseudospins: $(-1)^n \langle \tau_n^z \rangle \equiv \eta^z(\lambda) \neq 0$. At $\lambda_{c1} < \lambda < \lambda_{c2}$ the orbital degrees of freedom reveal their quantum nature: the onset of the spin Néel order ($\zeta \neq 0$) is accompanied by the emergence of the *transverse* component of the staggered pseudospin density: $(-1)^n \langle \tau_n^x \rangle \equiv \eta^x(\lambda) \neq 0$. Upon increasing λ, the staggered orbital order parameter $\boldsymbol{\eta}$ undergoes a continuous rotation from the z-direction to x-direction. At $\lambda = \lambda_{c2}$ a quantum Ising transition takes place in the orbital sector where η^z vanishes. At $\lambda > \lambda_{c2}$ both sectors are long-range ordered, with order parameters $\zeta, \eta^x \neq 0$. The dependence of order parameters on λ is schematically shown in Fig. 2(a); this picture is in full qualitative agreement with the results of the recent numerical studies.[22]

The crossover between the small and large λ limits studied in this section corresponds to path 1 on the phase diagram shown in Fig. 1. The path is located in the region $J_\tau \gg \Delta_S$. Starting from the massive phase I and moving

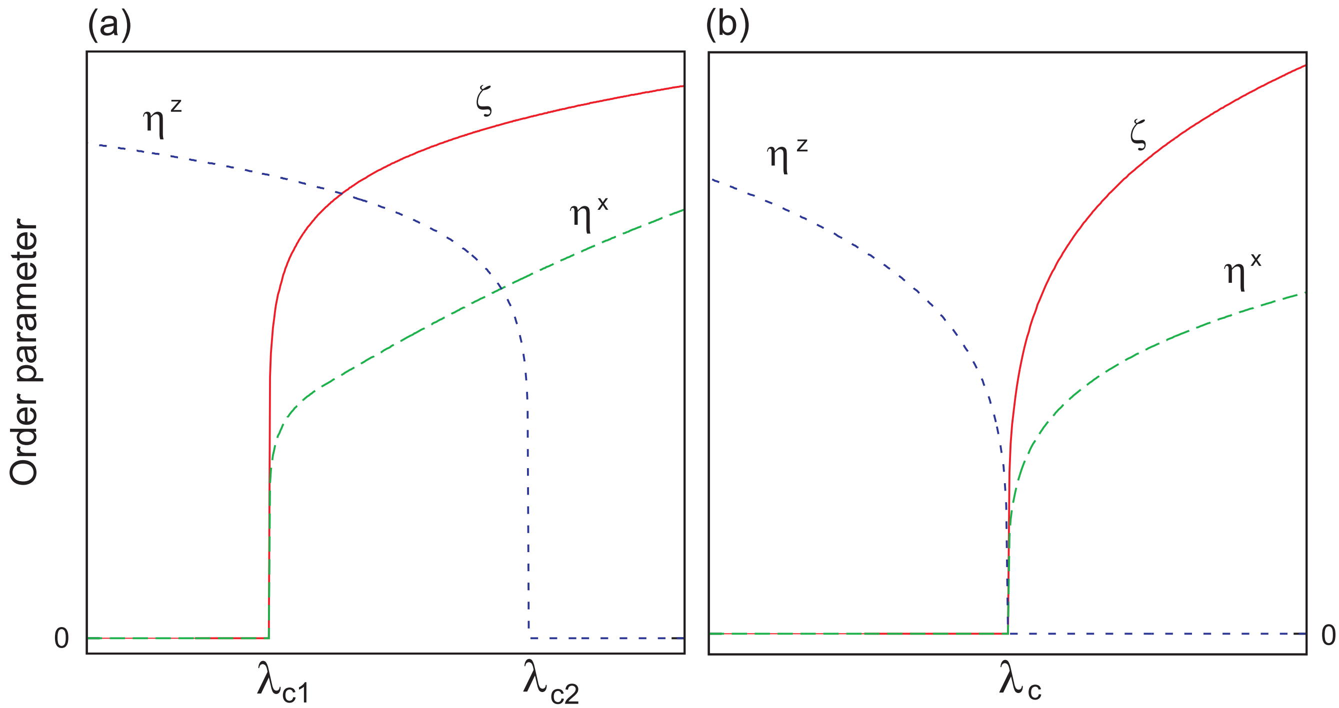

FIG. 2: Schematic diagram of order parameters as functions of the SO coupling constant λ. (a) Two Ising transitions in the $J_\tau \gg \Delta_S$ limit. (b) A single Gaussian transition in the $\Delta_S \gg J_\tau$ limit. These two scenarios correspond to path-1 and path-2 in the phase diagram (Fig. 1), respectively.

along this path we first observe the *spin-Ising* transition (I $\to$ II) to the Néel phase. Long-range ordering of the spins induces quantum reconstruction of the initialy classical orbital sector (i.e. generation of a nonzero η^x). The *orbital-Ising* transition (II $\to$ III) takes place inside the spin Néel phase. Of course, feedback effects (that is, orbit affecting spin) become inreasingly important upon deviating from the critical curve $\Delta_S J_\tau \sim 1$ into phases II and III, especially in the vicinity of the orbital transition where the spin-orbit coupling is very strong, $\lambda \sim J_\tau$. In this region the behavior of the spin degrees of freedom is not expected to follow that of an isolated anisotropic spin-1 chain in the Néel phase since the effect of an "explicit" staggered magnetic field $\sim \lambda\eta^x$ becomes important. We will see a pattern of such behavior in the opposite limit of "heavy" spins, which is discussed in the next section.

IV. GAUSSIAN CRITICALITY AT $J_\tau \ll \Delta_S$

In this section we turn to the opposite limiting case: $\Delta_S \gg J_\tau$. Now the spin degrees of freedom constitute the "fast" subsystem and can be integrated out to generate an effective action in the orbital sector. We will show that, in this regime, the intermediate massive phase where the orbital order parameter $\boldsymbol{\eta}$ undergoes a continuous rotation from $\boldsymbol{\eta} = (0,0,\eta^z)$ to $\boldsymbol{\eta} = (\eta^x,0,0)$ no longer exists. Going along path 2, Fig. 1, which is located in the region $\Delta_S \gg J_\tau$, we find that the two massive phases, I and III, are separated by a single Gaussian critical line characterized by central charge $c = 1$. On this line the vector $\boldsymbol{\eta}$ vanishes, the orbital degrees of freedom become gapless and represent a spinless Tomonaga-Luttinger liquid characterized by power-law orbital correlations.

At $\lambda = 0$ the spin-1 subsystem represents a disordered, isotropic spin liquid. Therefore the first nonzero correction to the low-energy effective action in the orbital sector appears in the second order in λ:

$$\begin{aligned} \Delta S_\tau^{(2)} &= -\frac{1}{6}\langle S_{S\tau}^2\rangle_S \\ &= -\frac{1}{2}\lambda^2 \sum_{nm}\int \mathrm{d}\tau_1 \int \mathrm{d}\tau_2\ \langle \mathbf{S}_n(\tau_1)\mathbf{S}_m(\tau_2)\rangle_S\ \tau_n^x(\tau_1)\tau_m^x(\tau_2), \end{aligned} \tag{28}$$

where $\langle\cdots\rangle_S$ means averaging over the massive spin degrees of freedom. According to the decomposition of the spin density, Eq. (4), the correlation function in (29) has the structure:

$$\langle \mathbf{S}_l(\tau)\mathbf{S}_0(0)\rangle = (-1)^l f_1(r/\xi_S) + f_2(r/\xi_S). \tag{29}$$

Here $\xi_s = v_s/\Delta_S$ is the spin correlation length and $\mathbf{r} = (v_s\tau, x)$ is the Euclidian two-dimensional radius-vector. f_1 and f_2 are smooth functions with the following asymptotic behaviour[27]

$$f_1(x) = C_1 x^{-1/2} e^{-x}, \quad f_2(x) = C_2 x^{-1} e^{-2x} \quad (x \gg 1), \tag{30}$$

where C_1 and C_2 are nonuniversal constants. DMRG calculations show[32] that $C_2 \ll C_1$; for this reason the contribution of the smooth part of the spin correlation function can be neglected in (29).

Integrating over the relative time $\tau_- = \tau_1 - \tau_2$ we find that the spin-orbit coupling generates a pseudospin xx-exchange with the following structure:

$$H'_\tau = \sum_n \sum_{l\geq 1} (-1)^{l+1} J'_\tau(l) \tau^x_n \tau^x_{n+l} \tag{31}$$

Here the exchange couplings exponentially decay with the separation l, $J'_\tau(l) \sim (\lambda^2/\Delta_S)\exp(-la_0/\xi_S)$, so the summation in (31) actually extends up to $l \sim \xi_S/a_0$. In the Heisenberg model ξ_S is of the order of a few lattice spacings, so for a qualitative understanding it would be sufficient to consider the $l = 1$ term as the leading one and treat the $l = 2$ term as a correction. Making a $\pi/2$ rotation in the pseudospin space, $\tau^z_n \to \tau^y_n$, $\tau^y_n \to -\tau^z_n$, we pass to the conventional notations and write down the effective Hamiltonian for the orbital degrees of freedom as a perturbed XY spin-1/2 chain:

$$H^{\rm eff}_\tau = \sum_n \left(J_x \tau^x_n \tau^x_{n+1} + J_y \tau^y_n \tau^y_{n+1} \right) + H'_\tau. \tag{32}$$

where

$$H'_\tau = -J'_x \sum_n \tau^x_n \tau^x_{n+2} + \cdots . \tag{33}$$

Here $J_y = J_\tau$, $J_x = J'_\tau(1) > 0$ and $J'_x = J'_\tau(2) > 0$. By order of magnitude $J'_x < J_x \sim \lambda^2/\Delta_S$.

In the absence of the perturbation H'_τ, the model (32) represents a spin-1/2 XY chain which for any nonzero anisotropy in the basal plane ($J_x \neq J_y$) has a Néel long-range order in the ground state and a massive excitation spectrum. This follows from the Jordan-Wigner transformation

$$\tau^z_n = 2a^\dagger_n a_n - 1, \quad \tau^+_n = \tau^x_n + \mathrm{i}\tau^y_n = 2a^\dagger_n e^{i\pi \sum_{j<n} a^\dagger_j a_j} \tag{34}$$

which maps the XY chain onto a model of complex spinless fermions with a Cooper pairing:[33]

$$\begin{aligned} H^{\rm eff}_\tau &= (J_x + J_y) \sum_n \left(a^\dagger_n a_{n+1} + h.c.\right) \\ &+ (J_x - J_y) \sum_n \left(a^\dagger_n a^\dagger_{n+1} + h.c.\right). \end{aligned} \tag{35}$$

By increasing λ (equivalently, decreasing J_τ) the model (35) can be driven to a XX quantum critical point, $J_x = J_y(1)$, i.e. $\lambda = \lambda_c \sim \sqrt{J_\tau \Delta_S}$, where the the system acquires a continuous U(1) symmetry. At this point the Jordan-Wigner fermions become massless and the system undergoes a continuous quantum transition.

The transition is associated with reorientation of the pseudospins. Away from the Gaussian criticality the effective orbital Hamiltoian is invariant under $Z_2 \times Z_2$ transformations: $\tau^x_n \to -\tau^x_n$, $\tau^z_n \to -\tau^z_n$. In massive phases this symmetry is spontaneously broken. Making a back rotation from τ^y to τ^z we conclude that at $J_y > J_x$ ($\lambda < \lambda_c$) $\eta^z \neq 0$, $\eta^x = 0$, while at $J_y < J_x$ ($\lambda > \lambda_c$) $\eta^z = 0$, $\eta^x \neq 0$. Both η^z and η^x vanish at the critical point, so contrary to the case $J_\tau \gg \Delta_S$, here there is no region of their coexistence.

The passage to the continuum limit for the model (32) based on Abelian bosonization is discussed in Appendix B. There we show that the perturbation H'_τ adds a marginal four-fermion interaction $g = J'_x(2)/\pi v \ll 1$ to the free-fermion model (B3). In the spin-chain language, this is equivalent to adding a weak ferromagnetic zz-coupling.

In the limit of weak XY anisotropy, $|\lambda - \lambda_c|/\lambda_c \ll 1$, the low-energy properties of the orbital sector are described by a quantum sine-Gordon model (all notations are explained in Appendix B)

$$\mathcal{H} = \frac{u}{2}\left[K\Pi^2 + \frac{1}{K}\left(\partial_x \Phi\right)^2\right] + \frac{2\gamma}{\pi\alpha}\cos\sqrt{4\pi}\Theta, \tag{36}$$

where

$$\gamma \sim J_\tau\left(\frac{\lambda-\lambda_c}{\lambda_c}\right), \quad K = 1 + 2g + O(g^2). \tag{37}$$

The U(1) criticality is reached at $\lambda = \lambda_c$ where, due to a finite value of g, the orbital degrees of freedom represent a Tomonaga-Luttinger liquid. Close to the criticality, the spectral gap in the orbital sector scales as the renormalized mass of the sine-Gordon model (36):

$$M_{\rm orb} \sim \left|\frac{\lambda-\lambda_c}{\lambda_c}\right|^{\frac{K}{2K-1}}. \tag{38}$$

Strongly fluctuating physical fields acquire coupling dependent scaling dimensions. In particular, according to the bosonization rules,[27] the staggered pseudospin densities are expressed in terms of the vertex operators,

$$\begin{aligned} (-1)^n \tau_n^x &\equiv n^x(x) \sim \sin\sqrt{\pi}\Theta(x), \\ (-1)^n \tau_n^z &\equiv n^z(x) \sim \cos\sqrt{\pi}\Theta(x), \end{aligned} \tag{39}$$

both with scaling dimension $d = 1/4K$. This anomalous dimension determines the power-law behaviour of the average staggered densities close to the criticality:

$$\begin{aligned} \eta^z(\lambda) &\sim (\lambda_c - \lambda)^{1/4K}, \quad \lambda < \lambda_c \\ \eta^x(\lambda) &\sim (\lambda - \lambda_c)^{1/4K}, \quad \lambda > \lambda_c. \end{aligned} \tag{40}$$

A finite staggered pseudospin magnetization η^x at $\lambda > \lambda_c$ generates an effective *external* staggered magnetic field in the spin sector:

$$H_S \to \bar{H} = H_S + H_S', \quad H_S' = -h_S\sum_n (-1)^n S_n^z, \tag{41}$$

where $h_S = -\lambda\eta^x$. The spectrum of the Hamiltonian $\bar{H}$ is always massive. This can be easily understood within the Majorana model (2). According to (6), in the continuum limit, the sign-alternating component of the spin magnetization, $N^3 \sim (-1)^n S_n^z$, can be expressed in terms of the order and disorder fields of the degenerate triplet of 2D disordered Ising models: $N^3 \sim \mu_1\mu_2\sigma_3$. In the leading order, the magnetic interaction H_S' gives rise to an effective magnetic field $h_3 = h_S\langle\mu_1\mu_2\rangle$ applied to the third Ising system: $h_3\sigma_3$. The latter always stays off-critical.

Since in the Haldane phase the spin correlations are short-ranged, close to the transition point the induced staggered magnetization ζ can be estimated using linear response theory. Therefore, at $0 < \lambda - \lambda_c \ll \lambda_c$, ζ follows the same power-law increase as that of η^x but with a smaller amplitude:

$$\zeta \sim \frac{h_S}{\Delta_S} \sim \left(\frac{J_\tau}{\Delta_S}\right)^{1/2}\left(\frac{\lambda-\lambda_c}{\lambda_c}\right)^{1/4K} \tag{42}$$

So, in the part of the phase C, Fig. 1, where $\Delta_S \gg J_\tau$, the η^x-orbital order, being the result of a spontaneous breakdown of a Z_2 symmetry $\tau_n^x \to -\tau_n^x$, acts as an effective staggered magnetic field applied to the spins and *induces* their Néel alignment. This fact is reflected in a coupling dependent, nonuniversal exponent $1/4K$ characterizing the increase of the staggered magnetization at $\lambda > \lambda_c$. The order parameters as functions of λ in the $\Delta_S \gg J_\tau$ limit is schematically shown in Fig. 2(b).

As already mentioned, the absence of a small parameter in the regime of strong hybridization, $J_\tau \sim J_S \sim \lambda$, makes the analysis of the phase diagram in this region not easily accessible by analytical tools. Nevertheless some plausible arguments can be put forward to comment on the topology of the phase diagram. It is tempting to treat the curve $J_\tau\Delta_S/\lambda^2 \sim 1$ as a single critical line going throughout the whole phase plane $(J_\tau/\lambda, \Delta_S/\lambda)$. If so, we then can expect that there exists a special singular point located in the region $J_\tau\Delta_S/\lambda^2 \sim 1$. This expectation is based on the fact that at $J_\tau \gg \Delta_s$ limit the transition is of the Ising type and the spontaneous spin magnetization below the critical curve follows the law $\zeta \sim (\lambda - \lambda_{c1})^{1/8}$ with a *universal* critical exponent, whereas at $J_\tau \ll \Delta_s$ the spin magnetization has a different, *nonuniversal* exponent, $\zeta \sim (\lambda - \lambda_c)^{1/4K}$. Continuity considerations make it very appealing to suggest that at the special point the Tomonaga-Luttinger liquid parameter takes the value $K = 2$, and the two power laws match. Since the central charges of two Ising and one Gaussian criticalities satisfy the relation $1/2 + 1/2 = 1$, the singular point must be a point where the two Ising critical curves merge into a single Gaussian one.

V. DYNAMICAL SIN SUSCEPTIBILITY AND NMR RELAXATION RATE IN THE VICINITY OF GAUSSIAN CRITICALITY

It may seem at the first sight that, in the regime $\Delta_S \gg J$, the spin degrees of freedom which have been integrated out remain massive across the orbital Gaussian transition, and the spectral weight of the staggered spin fluctuations is only nonzero in the high-energy region $\omega \sim \Delta_S$. However, this conclusion is only correct for the zeroth-order definition of the spin field $\mathbf{N}_0(x)$, given by Eq. (6), with respect to the spin-orbit interaction. In fact, the staggered magnetization hybridizes with low-energy orbital modes via SO coupling already in the first order in λ and thus acquires a low-energy projection which contributes to a nonzero spectral weight displayed by the dynamical spin susceptibility at energies well below the Haldane gap.

To find the low-energy projection of the field $N^z(\mathbf{r})$, we must fuse the local operator $N^z_0(\mathbf{r})$ with the perturbative part of the total action. Keeping in mind that close to and at the Gaussian criticality most strongly fluctuating fields are the staggered components of the orbital polarization, we approximate the SO part of the Euclidian action by the expression

$$S_{S\tau} \simeq \frac{\lambda a_0}{v_S} \int \mathrm{d}^2\mathbf{r}\ N^z(\mathbf{r}) n^x(\mathbf{r}), \tag{43}$$

where $\mathbf{r} = (v_S\tau, x)$ is the two-dimensional radius vector (here τ is the imaginary time). We thus construct

$$\begin{aligned} N^z_P(\mathbf{r}) &= \langle e^{-S_{S\tau}} N^z(\mathbf{r})\rangle \\ &= N^z_0(\mathbf{r}) - \frac{\lambda a_0}{v_S}\int \mathrm{d}^2\mathbf{r}_1 \langle N^z_0(\mathbf{r}) N^z_0(\mathbf{r}_1)\rangle_S\ n^x(\mathbf{r}_1) \\ &\quad +\ O(\lambda^2), \end{aligned} \tag{44}$$

where averaging is done over the unperturbed, high-energy spin modes. For simplicity, here we neglect the anisotropy of the spin-liquid phase of the S=1 chain and use formula (8). The spin correlation function is short-ranged. Treating the spin correlation length $\xi_S \sim v_S/\Delta_S$ as a new lattice constant (new ultraviolet cutoff) and being interested in the infrared asymptotics $|\mathbf{r}| \gg \xi_S$, we can replace in (44) $n^x(\mathbf{r}_1)$ by $n^x(\mathbf{r})$. The integral

$$\begin{aligned} &\int \mathrm{d}^2\boldsymbol{\rho}\ \langle N^z_0(\boldsymbol{\rho}) N^z_0(\mathbf{0})\rangle_S \\ &\sim \frac{1}{a_0^2}(a/\xi_S)^{3/4}\int_0^\infty d\rho\ \rho\sqrt{\xi_s/\rho}\ e^{-\rho/\xi_S} \sim (\xi_S/a_0)^{5/4}. \end{aligned} \tag{45}$$

So the first-order low-energy projection of the staggered magnetization is proportional to

$$N^z_P(\mathbf{r}) \sim \frac{\lambda}{\Delta_S}\left(\frac{\xi_S}{a_0}\right)^{1/4} n^x(\mathbf{r}). \tag{46}$$

This result clarifies the essence of the hybridization effect: close to the Gaussian criticality the spin fluctuations acquire a finite spectral weight in the low-energy region, $\omega \ll \Delta_S$, $q \sim \pi$, which is contributed by orbital fluctuations and can be probed in magnetic inelastic neutron scattering experiments and NMR measurements.

Away from but close to the Gaussian criticality the behavior of the dynamical spin susceptibility $\Im m\chi(q,\omega)$ is determined by the excitation spectrum of the sine-Gordon model for the dual field, Eq.(36). Since $K > 1$, it consists of kinks, antikinks carrying the mass M_{orb}, and their bound states (breathers) with masses (see e.g. Ref. 27)

$$\begin{aligned} &M_j = 2M_{\mathrm{orb}}\sin(\pi j/2\nu), \\ &j = 1, 2, \ldots \nu - 1, \quad \nu = 2K - 1 \end{aligned} \tag{47}$$

Since $K - 1 = 2g$ is small, there will be only the first breather in the spectrum, with mass $M_1 = 2M_{\mathrm{orb}}(1 - 2\pi^2 g^2)$. The sine-Gordon model is integrable, and the asymptotics of its correlation functions in the massive regime have been calculated using the form-factor approach (see for a recent review 35). Here we utilize some of the known results. At $\lambda < \lambda_c$ the operator $n^x \sim \sin\sqrt{\pi}\Theta$ has a nonzero matrix element between the vacuum and the first breather state. This form-factor contributes to a coherent peak in the dynamical spin susceptibility at frequencies much smaller than than the Haldane gap:

$$\begin{aligned} \Im m\chi(q,\omega,T=0) \ &= \ A(\lambda/\Delta_S)^2\delta[\omega^2 - (q-\pi)^2 v^2 - M_1^2] \\ &\quad +\ \Im m\chi_{\mathrm{cont}}(q,\omega,T=0). \end{aligned} \tag{48}$$

Here A is a constant and the second term is the contribution of a multi-kink continuum of states with a threshold at $\omega = 2M_{\rm orb}$. At $\lambda > \lambda_c$ the spectral properties of the operator $\cos\sqrt{\pi}\Theta$ coincide with those of the operator $\sin\sqrt{\pi}\Theta$ at $\lambda < \lambda_c$. For symmetry reasons[35], this operator does not couple to the first breather, so that at $\lambda > \lambda_c$ $\Im m\chi(q,\omega)$ will only display the kink-antikink scattering continuum.

We see that, due to spin-orbit hybridization effects, the spin sector of our model loses the properties of a spin liquid already in a noncritical orbital regime. This tendency gets strongly enhanced at the orbital Gaussian criticality ($M_{\rm orb} \to 0$) where all multi-particle processes merge, and the spin correlation function exhibits an algebraically decaying asymptotics

$$\langle N^z(\mathbf{r})N^z(\mathbf{0})\rangle \simeq \langle N^z_P(\mathbf{r})N^z_P(\mathbf{0})\rangle \sim \left(\frac{\lambda}{\Delta_S}\right)^2 \left(\frac{a}{r}\right)^{\frac{1}{2K}}, \tag{49}$$

implying that the spin sector of the model becomes reminiscent of Tomonaga-Luttinger liquid. In this limit (here for simplicity we consider the $T = 0$ case) the dynamical spin susceptibility is given by[34]

$$\Im m\chi(q,\omega,T=0) \sim (\lambda/\Delta_S)^2 \left[\omega^2 - v^2(q-\pi)^2\right]^{\frac{1}{4K}-1}. \tag{50}$$

The NMR relaxation rate probes the spectrum of local spin fluctuations

$$\frac{1}{T_1} = A^2 T \lim_{\omega\to 0}\frac{1}{\omega}\sum_q \Im m\chi^{zz}(q,\omega,T)$$

where A is an effective hyperfine constant. In spin-liquid regime of an isolated spin-1 chain, the existence of a Haldane gap makes $1/T_1$ exponentially suppressed[36]: $1/T_1 \sim \exp(-2\Delta_S/T)$. The admixture of low-energy orbital states in the spin-fluctuation spectrum drastically changed this result. A simple power counting argument[37] leads to a power-law temperature dependence of the NMR relaxation rate:

$$\frac{1}{T_1} \sim A^2 \left(\frac{\lambda}{\Delta_s}\right)^2 T^{\frac{1}{2K}-1} \tag{51}$$

This result is valid not only exactly at the Gaussian criticality but also in its vicinity provided that the temperature is larger than the orbital mass gap. By construction (see the preceding section) $K \geq 1$. This means that the exponent $1/2K - 1$ is *negative* and the NMR relaxation rate *increases* on lowering the temperature. It is worth noticing that such regimes are not unusual for Tomonaga-Luttinger phases of frustrated spin-1/2 ladders.[38] For our model, such behavior of $1/T_1$ would be a strong indication of an extremely quantum nature of the collective orbital excitations.[39]

VI. BEHAVIOR IN A MAGNETIC FIELD: QUANTUM ISING TRANSITION IN ORBITAL SECTOR

We have seen in Sec.III that, due to spin-orbit coupling, the Néel ordering of the spins is accompanied by the emergence of quantum effects in the orbital sector: the classical orbital Ising chain transforms to a quantum one. In this section we briefly comment on a similar situation that can arise upon application of a uniform external magnetic field h.

Since the spin-1 chain is massive, it will acquire a finite ground-state magnetization $\langle S^z\rangle$ only when the magnetic field, h, is higher than the critical value $h_{c1} \sim \Delta_S$, corresponding to the commensurate-incommensurate (C-IC) transition. According to the definition (5), a uniform magnetic field along the z-axis, $\mathcal{H}_{\rm mag} = -hI^z$, mixes up a pair of Majorana fields, ξ^1 and ξ^2, and splits the spectrum of $S^z = \pm 1$ excitations (the $S^z = 0$ modes are unaffected by the field). At $h = h_{c1}$ the gap in the spectrum of the $S^z = 1$ excitations closes, and at $h > h_{c1}$ these modes condense giving rise to a finite magnetization. Once $\langle S^z\rangle \neq 0$, the effective Hamiltonian of the τ-chain becomes

$$\bar{H}_\tau = J_\tau \sum_n \tau^z_n \tau^z_{n+1} - \Delta_\tau \sum_n \tau^x_n, \qquad \Delta_\tau = \lambda\langle S^z\rangle. \tag{52}$$

Here we ignore the fluctuation term that couples τ^x_n to $\Delta S^z_n = S^z_n - \langle S^z_n\rangle$.

One should keep in mind that there exists the second C-IC transition at a higher field h_{c2} associated with full polarization of the spin-1 chain. To simplify further analysis, let us assume that the range of magnetic fields $h_{c1} < h < h_{c2}$, where an isolated spin-1 chain has an incommensurate, gapless ground state, is sufficiently broad. This can be easily achieved in the biquadratic model (3) with $\beta \sim 1$, in which case the Haldane gap – and hence h_{c1} – is small, and the effects associated with the second C-IC transition can be neglected.

Now, by increasing the magnetic field h in the region $h > h_{c1}$, the effective orbital chain (52) can be driven to an Ising criticality. The induced transverse "magnetic field" Δ_τ is proportional to a nonzero magnetization of the spin-1 chain. If λ/J_τ is large enough, then upon increasing the field the effective quantum Ising chain (52) can reach the point $\Delta_\tau(h^*) = J_\tau$ where the Ising transition occurs. This will happen at some field $h = h^* > h_{c1}$. In the region $|h - h^*|/h^* \ll 1$ the quantum Ising τ-chain will be slightly off-critical. Due to the SO coupling, these massive orbital excitations will interact with the gapless $S^z = \pm 1$ spin modes. However, this interaction can only give rise to the orbital mass renormalization (i.e. a small shift of the Ising critical point) and a group velocity renormalization of the spin-doublet modes. For this reason we do not expect the aforementioned spin-orbital fluctuation term to cause any qualitative changes.

The above discussion reveals an interesting fact: a sufficiently strong magnetic field acting on the spin degrees of freedom can affect the orbital structure of the chain and drive it to a quantum Ising transition. The difference with the situation discussed in Sec.III is that the external magnetic field induces a uniform spin polarization which, in turn, gives rise to a uniform transverse orbital ordering $\langle \tau^x_n \rangle \neq 0$. Thus, the classical long-range orbital order $\langle \tau^z_n \rangle = (-1)^n \eta^z$, present at $h < h^*$, disappears in the region $h > h^*$, where the orbital degrees of freedom are characterized by a transverse ferromagnetic polarization, $\langle \tau^x \rangle \neq 0$.

VII. CONCLUSION AND DISCUSSION

In this paper, we have proposed and analyzed a 1D spin-orbital model in which a spin-1 Haldane chain is locally coupled to an orbital Ising chain by an on-site term $\lambda\, \tau^x S^z$ originating from relativistic spin-orbit (SO) interaction. The SO term not only introduces anisotropy to the spin sector, but also gives quantum dynamics to the orbital degrees of freedom. We approach this problem from well defined limits where either the spin or the orbital sector is strongly gapped and becomes a 'fast' subsystem which can be integrated out. By analyzing the resultant effective action of the remaining 'slow' degrees of freedom, we have identified the stable massive and critical phases of the model which are summarized in a schematic phase diagram shown in Fig. 1.

In the limit dominated by a large orbital gap, i.e. $J_\tau \gg \Delta_S$, integrating out the orbital variables gives rise to an easy-axis spin anisotropy $D(S^z)^2$ where $D \sim -\lambda^2/J_\tau$. As λ increases, the disordered Haldane spin liquid undergoes an Ising transition into a magnetically ordered Néel state. The presence of antiferromagnetic spin order ζ in the Néel phase in turn generates an effective transverse field $h \sim \lambda\zeta$ acting on the orbital Ising variables. The orbital sector which is described by the Hamiltonian of a quantum Ising chain reaches criticality when $h = J_\tau$. In between the two Ising critical points lies an intermediate phase (phase II in Fig. 1) where both Ising order parameters η^x and η^z are nonzero. Such a two-stage ordering scenario illustrated by path 1 in the phase diagram (Fig. 1) has been confirmed numerically by recent DMRG calculations.[22] Interestingly, the orbital Ising transition can also be induced by applying a magnetic field to the spin sector. As the field strength is greater than the Haldane gap, a field-induced magnon condensation results in a finite magnetization density $\langle S^z \rangle$ in the linear chain. Thanks to the SO coupling, the orbital sector again acquires a transverse field $h \sim \lambda \langle S^z \rangle$ and becomes critical when $h = J_\tau$.

A distinct scenario of the orbital reorientation transition $\eta^z \to \eta^x$ occurs in the opposite limit $\Delta_S \gg J_\tau$. This time we integrate out the fast spin subsystem and obtain a perturbed spin-1/2 XY Hamiltonian for the orbital sector. The effective exchange constants are given by $J_x \sim \lambda^2/\Delta_S$ and $J_y = J_\tau$. As λ is varied, the orbital sector reaches a Gaussian critical point when $J_x = J_y$, at which the system acquires an emergent U(1) symmetry. The orbital order parameter goes directly from $\boldsymbol{\eta} = (0, 0, \eta^z)$ to $(\eta^x, 0, 0)$ in this single-transition scenario (illustrated by path 2 in Fig. 1). Both order parameters η^x and η^z vanish at the critical point. We have shown that spin-orbital hybridization effects near the Gaussian transition lead to the appearance of a non-zero spectral weight of the staggered spin density well below the Haldane gap – the effect which can be detected by inelastic neutron scattering experiments and NMR measurements.

The stability analysis of the orbital Gaussian criticality in the original lattice model (1), done in Appendix B, has shown that this critical regime is protected by the $\tau^z \to -\tau^z$ symmetry of the underlying microscopic model. This symmetry will be broken in the presence of an orbital field $\delta \sum_n \tau^z_n$ which removes degeneracy between the local orbitals d_{zx} and d_{yz} and adds a "magnetic" field along the y-axis in the effective XY model (32). Such perturbation will drive the orbital sector away from the Gaussian criticality. The same argument applies to a perturbation with the structure $\beta \sum_n S^z_n \tau^z_n$ which also breaks the aforementioned symmetry. Integrating over the spins will generate an extra term $\sim \lambda\beta \sum_n (\tau^x_n \tau^y_{n+1} + \tau^y_n \tau^z_{n+1})$ which, in the continuum limit, translates to $\lambda\beta \sin\sqrt{4\pi}\Theta$. As explained in Appendix B, such perturbation will keep the orbital sector gapped with coexisting η^x and η^z orderings.

Since the analysis presented in this paper is done in the limiting cases, precise predictions on the detailed shape of the phase diagram or on the behavior of correlation functions in the regime of strong hybridization of spin and orbital degrees of freedom, where all interactions included in the model are of the same order, are beyond our reach and require further numerical calculations. On the other hand, the continuity and scaling analysis allow us to believe that the global topology of the phase diagram and character of critical lines are given correctly. Finally the spin-orbital model Eq. (1) can be generalized to the zigzag geometrical where two parallel spin-1 chains are coupled to a zigzag Ising orbital chain via on-site SO interaction. The zigzag case is closely related to the quasi-1D compound CaV_2O_4. While the two-Ising-transitions scenario is expected to hold in the $J_\tau \gg \Delta_S$ regime, the counterpart of Gaussian criticality in the zigzag chain remains to be explored and will be left for future study.

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Appendix A: Ising correlation function

In this Appendix we estimate the correlation function $\Gamma^{xx}_{nm}(\tau) = \langle \tau^x_n(\tau)\tau^x_m(0)\rangle$, where the averaging is performed over the ground state of the Ising Hamiltonian $H_\tau = J_\tau \sum_n \tau^z_n \tau^z_{n+1}$, and $\tau^x_n(\tau) = e^{\tau H_\tau}\tau^x_n e^{-\tau H_\tau}$.

It proves useful to make a duality transformation:

$$\tau^z_n \tau^z_{n+1} = \mu^x_n, \quad \tau^x_n = \mu^z_n \mu^z_{n+1}.$$

The new set of Pauli matrices μ^a_n represents disorder operators. The Hamiltonian and correlation function become:

$$H \to J_\tau \sum_n \mu^x_n, \tag{A1}$$

$$\Gamma^{zz}_{nm}(\tau) \to \langle \mu^z_n(\tau)\mu^z_{n+1}(\tau)\mu^z_m(0)\mu^z_{m+1}(0)\rangle. \tag{A2}$$

The most important fact about the dual representation is the additive, single-spin structure of the Hamiltonian: the latter describes noninteracting spins in an external "magnetic field" J_τ. Notice that by symmetry $\langle \mu^z_n \rangle = 0$. Therefore the correlation function in (A2) has an ultralocal structure:

$$\Gamma^{xx}_{nm}(\tau) = \delta_{nm} Y^2(\tau), \quad Y(\tau) = \langle \mu^z_n(\tau)\mu^z_n(0)\rangle. \tag{A3}$$

The time-dependence of the disorder operator can be explicitly computed,

$$\mu^z_n(\tau) = e^{\tau J_\tau \mu^x_n} \mu^z_n e^{-\tau J_\tau \mu^x_n} = \mu^z_n \cosh(2J_\tau \tau) - \mathrm{i}\mu^y_n \sinh(2J_\tau \tau).$$

Therefore (below we assume that $\tau > \tau'$)

$$\begin{aligned} Y(\tau - \tau') &= \cosh 2J_\tau(\tau - \tau') + \langle \mu^x \rangle \sinh 2J_\tau(\tau - \tau') \\ &= \exp[-2|J_\tau|(\tau - \tau')]. \end{aligned} \tag{A4}$$

Here we used the fact that, in the ground state the Hamiltonian H_τ, $\langle \mu^x \rangle = -\mathrm{sgn}\ J_\tau$. Thus, as expected for the 1D Ising model, the correlation function $\Gamma^{xx}_{nm}(\tau)$ is local in real space and decays exponentially with τ:

$$\Gamma^{xx}_{nm}(\tau) = \delta_{nm} \exp\left(-4J_\perp|\tau|\right). \tag{A5}$$

Appendix B: Perturbed XY chain, Eq. (32)

In this Appendix we analyze the perturbation (33) to the XY spin chain (32) and show that at the XX point it represents a marginal perturbation which transforms the free-fermion regime to a Gaussian criticality describing a Luttinger-liquid behavior of the orbital degrees of freedom.

Using the Jordan-Wigner transformation (34) we rewrite (33) as $H'_\tau = H'_1 + H'_2$, where

$$H'_1 = \frac{J'_x(2)}{2}\sum_n (a_n^\dagger a_{n+2} + h.c.)(a_{n+1}^\dagger a_{n+1} - \frac{1}{2}), \tag{B1}$$

$$H'_2 = \frac{J'_x(2)}{2}\sum_n (a_n^\dagger a_{n+2}^\dagger + h.c.)(a_{n+1}^\dagger a_{n+1} - \frac{1}{2}). \tag{B2}$$

Assuming that $|J_x - J_y|, J'_x \ll J_x + J_y$, we pass to a continuum description of the XY chain in terms of chiral, right (R) and left (L), fermionic fields based on the decomposition (to simplify notations we set here $a_0 = 1$): $a_n \to (-\mathrm{i})^n R(x) + \mathrm{i}^n L(x)$. Then the Hamiltonian density of the XY model takes the form:

$$\mathcal{H}_{XY}(x) = -\mathrm{i}v\left(R^\dagger \partial_x R - L^\dagger \partial_x L\right) - 2\mathrm{i}\gamma\left(R^\dagger L^\dagger - h.c.\right), \tag{B3}$$

where $\gamma = J_x - J_y$. Standard rules of Abelian bosonization[27] transform (B3) to a quantum sine-Gordon model:

$$\mathcal{H}_{XY}(x) = \frac{v}{2}\left[\Pi^2 + (\partial_x\Phi)^2\right] + \frac{2\gamma}{\pi\alpha}\cos\sqrt{4\pi}\Theta, \tag{B4}$$

where $v = 2(J_x + J_y)a_0$ is the Fermi velocity, $\Pi(x) = \partial_x\Theta(x)$ is the momentum conjugate to the scalar field $\Phi(x) = \Phi_R(x)+\Phi_L(x)$, and $\Theta(x) = -\Phi_R(x)+\Phi_L(x)$ is the field dual to $\Phi(x)$. Here $\Phi_{R,L}(x)$ are chiral components of the scalar field. Using the fact that the fermions are spinless, one can impose the condition $[\Phi_R(x), \Phi_L(x')] = i/4$ and thus make sure that the bosonization rules correctly reproduce the anticommutation relations $\{R(x), L(x')\} = \{R(x), L^\dagger(x')\} = 0$. An explicit introduction of the so-called Klein factors becomes necessary when bosonizing fermions with an internal degree of freedom, such as spin 1/2, chain index *etc*, which is not the case here.

Let is find the structure of the perturbation (33) in the continuum limit. First of all we notice that

$$\begin{aligned} a_{n+1}^\dagger a_{n+1} - 1/2 \equiv\ & :a_{n+1}^\dagger a_{n+1}: \\ \to & (:R^\dagger R: + :L^\dagger L:) + (-1)^{n+1}(R^\dagger L + L^\dagger R) \\ = & \frac{1}{\sqrt{\pi}}\partial_x\Phi + \frac{(-1)^n}{\pi\alpha}\sin\sqrt{4\pi}\Phi. \end{aligned} \tag{B5}$$

Similarly

$$\begin{aligned} & a_n^\dagger a_{n+2} + h.c. \\ & \to -2\left[(:R^\dagger R: + :L^\dagger L:) + (-1)^n(R^\dagger L + L^\dagger R)\right] \\ & = -2\left[\frac{1}{\sqrt{\pi}}\partial_x\Phi - \frac{(-1)^n}{\pi\alpha}\sin\sqrt{4\pi}\Phi\right]. \end{aligned} \tag{B6}$$

Dropping Umklapp processes $R^\dagger(x)R^\dagger(x+\alpha)L(x+\alpha)L(x) + h.c. \sim \cos\sqrt{16\pi}\Phi$ as strongly irrelevant (with scaling dimension 4) at the XX criticality and ignoring interaction of the fermions in the vicinity of the same Fermi point, we find that

$$\begin{aligned} & (a_n^\dagger a_{n+2} + h.c.)(a_{n+1}^\dagger a_{n+1} - 1/2)\Big|_{\text{smooth}} \\ & \to -8 :R^\dagger R::L^\dagger L: = 2\left[\Pi^2 - (\partial_x\Phi)^2\right]. \end{aligned} \tag{B7}$$

We see that the perturbation H'_1 generates a marginal four-fermion interaction to the free-fermion model (B3), thus transforming the model (32) to an XYZ model with a weak ferromagnetic (zz)-coupling. This interaction can be incorporated into the Gaussian part of the bosonic theory (B4) by changing the compactification radius of the field Φ:

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{XY} + \mathcal{H}'_1 \\ &= \frac{u}{2}\left[K\Pi^2 + \frac{1}{K}(\partial_x\Phi)^2\right] - \frac{2\gamma}{\pi\alpha}\cos\sqrt{4\pi}\Theta. \end{aligned} \tag{B8}$$

Here u is the renormalized velocity and K is the interaction constant which at $J_x' \ll (J_x+J_y)$ is given by $K = 1 + 2g + O(g^2)$, where $g = J_x'(2)a_0/\pi v \ll 1$.

Now we turn to H_2'. We have:

$$\begin{aligned} & a_n^\dagger a_{n+2}^\dagger + h.c. \\ & \to - \left[R^\dagger(x)L^\dagger(x+\alpha) + L^\dagger(x)R^\dagger(x+\alpha) + h.c.\right] \\ & \ +(-1)^n \left[R^\dagger(x)R^\dagger(x+\alpha) + L^\dagger(x)L^\dagger(x+\alpha) + h.c.\right]. \end{aligned} \tag{B9}$$

Bosonizing the smooth term in the r.h.s. of (B10) one obtains $\partial_x\Phi \cos\sqrt{4\pi}\Theta$. Bosonizing the staggered term yields $\sin\sqrt{4\pi}\Phi\cos\sqrt{4\pi}\Theta$. Using the OPE

$$\begin{aligned} & \sin\sqrt{4\pi}\Phi(x)\sin\sqrt{4\pi}\Phi(x+\alpha) \\ & \qquad = \text{const} - \pi\alpha^2(\partial_x\Phi)^2 - \frac{1}{2}\cos\sqrt{16\pi}\Phi, \end{aligned}$$

we find that, in the continuum limit, the Hamiltonian density $\mathcal{H}_2'$ is contributed by the operators $\cos\sqrt{4\pi}\Theta$ and $(\partial_x\Phi)^2\cos\sqrt{4\pi}\Theta$ (as before, we drop corrections related to Umklapp processes). The former leads to a small additive renormalization of the fermionic mass γ and thus produces a shift of the critical point. The latter represents an irrelevant perturbation (with scaling dimension 3) at the XX criticality. In a noncritical regime it renormalizes the mass and four-fermion coupling constant g.

Considering the structure of the remaining terms in the expansion (31) one arrives at similar conclusions. Here a remark is in order. The only dangerous perturbation which would dramatically affect the above picture is $\sin\sqrt{4\pi}\Theta$. The presence of two nonlinear terms in the Hamiltonian, $\gamma\cos\sqrt{4\pi}\Theta + \delta\sin\sqrt{4\pi}\Theta$, would make the fermionic mass equal to $\sqrt{(\lambda-\lambda_c)^2+\delta^2}$. The Gaussian criticality in this case would never be reached, the model would always remain massive, and nonzero staggered pseudospin densities, η^z and η^x, would coexist in the whole parameter range of the model.

Fortunately, the appearance of the operator $\sin\sqrt{4\pi}\Theta$ is forbidden by symmetry. The initial Hamiltonian (1) is invariant under global pseudospin inversion In the z-component only: $\tau_n^z \to -\tau_n^z$. After rotation $\tau^z \to \tau^y$ this translates to $\tau_n^y \to -\tau_n^y$. Using the bosonized expressions (39) for the staggered pseudospin densities we find that the corresponding transformation of the dual field is $\Theta \to \sqrt{\pi} - \Theta$ and so the bosonized Hamiltonian density must be invariant under this transfomation. This explains why the operator $\sin\sqrt{4\pi}\Theta$ cannot appear in the effective continuum theory.

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