AB_2 Hubbard chains in the strong-coupling limit: Ferrimagnetism, Nagaoka and RVB states, phase separation, and Luttinger-liquid behavior

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We present a functional-integral formalism suitable to describe the strong-coupling regime below half filling of AB_2 Hubbard chains, with experimental realizations in inorganic and organic polymeric compounds. At half filling (one electron per site: $\delta=0$), we obtain the long-range-ordered ferrimagnetic ground state and correctly reproduce the associated quantum nonrelativistic nonlinear σ model, with presence of topological Wess-Zumino terms, which has been also found in a coherent-state representation, restricted however to treat the case of localized spins. A fully polarized (Nagaoka) ferromagnetic state is obtained in the infinite-coupling regime near half filling, and at doping $\delta=1/3$ (two electrons per unit cell) insulating short-range resonating-valence-bond (RVB) singlet states take place. Competition between Nagaoka and RVB mechanisms can lead to phase separation for $0<\delta<1/3$. By increasing the hole doping, a crossover regime for $1/3<\delta<2/3$ anticipates the emergence of Luttinger-liquid behavior for $\delta\geq 2/3$. In particular, at $\delta=2/3$ (one electron per cell) the system behaves similarly to a critical spin-1/2 antiferromagnetic linear chain. All these results find support in numerical studies both in the half filling and doped regimes.

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I. INTRODUCTION

The understanding and precise characterization of low-temperature (low-T) magnetism and electronic correlations in quasi-one-dimensional (quasi-1D) compounds still offer great challenges despite the recent progress.[1] Difficulties arise, e.g., related to the special unit-cell topology present in such low-dimensional systems and/or to the existence of correlated p electrons of light elements, such as C, O, and N, in contrast to the conventional magnetism found in transition and rare-earth metals, with partially filled d or f orbitals. Suitable examples are provided by inorganic and organic ferrimagnetic compounds with AB_2 unit-cell structure[2] (see Fig. 1), modeled by the Hubbard Hamiltonian. On the inorganic side, realizations include homometallic compounds[3] with a line of trimer clusters characteristic of phosphates of formula $A_3Cu_3(PO_4)_4$, where A=Ca, Sr, and Pb. Also, the frustrated AB_2 (azurite) compound[4] $Cu_3(CO_3)_2(OH)_2$ displays low-T short-range magnetic order, suitably described by a distorted diamond chain model. On the other hand, low-T ferrimagnetism can be also found[5] in the organic compound with AB_2 structure 2-[3′, 5′-bis(*N-tert*-butylaminoxyl) phenyl]-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl 3-oxide, or PNNBNO. In a broader perspective, these chains might represent a relevant alternative route to reaching two-dimensional (2D) low-T quantum physics from quasi-1D systems.[6,7]

Topology of the unit cell is a key factor underlying the magnetism in bipartite AB_2 Hubbard chains. Indeed, a rigorous theorem by Lieb[8] asserts that these systems, with one electron per site on average (half-filled limit) and any repulsive Coulombian interaction $U>0$, present mean ground-state spin per unit cell $\hbar/2$. The presence of quantum ferrimagnetic long-range order at $T=0$ is shown[8,9] to be intrinsically related to the existence of a macroscopically degenerate flat band due to the AB_2 topology, with a Hubbard gap U to the high-energy modes, which is absent in linear Hubbard chains.[10–12] In this context, much has been reported on the analytical properties of AB_2 Hubbard chains precisely at half filling, in which a map onto the AB_2 Heisenberg model applies[13–17] in the strong-coupling limit, and connections can be also established with quantum nonrelativistic nonlinear σ,[17] quantum spherical,[18] t-J,[6] and quantum rotor[19] models.

In contrast to the half-filled scenario, an analytical approach away from half filling is still lacking for AB_2 Hubbard chains, beyond Hartree-Fock level.[9] Indeed, most of the progress in the doped regime has been achieved through quantum Monte Carlo,[9] exact diagonalization (ED),[9,13,20–22] Lanczos,[20] and density-matrix renormalization-group (DMRG) (Refs. 6, 20, and 22) numerical methods. These works have pointed to a rich phase diagram as a function of the electron density (doping) and Coulombian coupling, which remains virtually unexplored from the analytical viewpoint. For instance, in the weak-coupled slightly underdoped region the ferrimagnetic phase has been shown[20] to sustain up to hole concentration $\delta\approx 0.02$ (with respect to half filling $\delta\equiv 1-N_e/N=0$, where N_e and N are the number of electrons and sites, respectively); on the other hand, for $0.02<\delta$

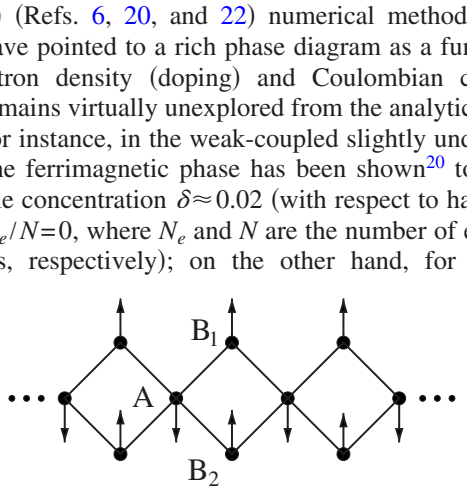

FIG. 1. AB_2 Hubbard chain, displaying one of the twofold-degenerate (with respect to spin inversion) ground-state ferrimagnetic configurations in the half-filled strong-coupling limit.

<0.07 hole itinerancy promotes incommensurate spin correlations (a spiral phase), with a δ-dependent peak position in the magnetic structure factor. In the infinite-coupling regime with one hole a fully polarized ground state is set[20] due to hole itinerancy as well (Nagaoka mechanism[11,23]), in contrast to the ferrimagnetic ground state observed precisely at half filling (Lieb's theorem). The strong-coupled Nagaoka ferromagnetic phase has been also observed[9,20] for doping $\delta < \delta_{PS}(\infty) \approx 0.225$, with the spin ordering displaying spatially modulated profiles on top of the polarized state. For higher doping, a phase separation (PS),[9,20,24] into coexisting insulating and metallic states emerges for $\delta_{PS}(U) < \delta < 1/3$, respectively associated with even (singlet) and odd (triplet) local parity symmetry of the ground state. At the upper bound of the phase-separated regime, $\delta=1/3$, the system becomes a Mott insulator, with spin and charge gaps, very short-ranged correlations, and can be well described[20] by a resonating-valence-bond (RVB) picture.[10,25–27] A crossover region sets for $1/3 < \delta < 2/3$, while a Luttinger-liquid behavior[28] has been characterized for $\delta \geq 2/3$.[20] In particular, for commensurate doping $\delta=2/3$ the system is an insulator, with gapless spin excitation, charge gap vanishing as a function of the Coulombian repulsion and critical behavior of the spin-spin correlation function, similarly to the strong-coupled Hubbard model in a linear chain at half filling.[10,29,30]

In this work we provide a functional-integral representation suitable to describe the strong-coupling limit of quantum AB_2 Hubbard chains in the doped regime. As the quasi-1D AB_2 unit-cell structure is taken into account explicitly into the formalism, remarkable differences with respect to the linear Hubbard chains manifest ubiquitously in mathematical as well as in physical terms, both at half filling and in the doped regime. As an important check to the theory, the effective low-lying Lagrangian at half-filled band correctly reproduces the long-range-ordered ferrimagnetic ground state and the associated quantum nonrelativistic nonlinear σ model, with presence of topological Wess-Zumino terms, which has been also obtained[17] in a spin-based coherent-state representation,[10] of applicability restricted to localized spins. Further, in the infinite-coupling regime we also find Nagaoka and RVB states, respectively near half filling and at $\delta=1/3$, with phase separation for intermediate doping, as well as Luttinger-liquid behavior for $\delta \geq 2/3$, with charge and spin degrees of freedom decoupled, in agreement with numerical findings.[9,20] We mention that the present formalism can, in principle, be applied to treat higher dimensionality systems with AB_2 unit cell. In this context, when considering AB_2 structures in higher dimensions one should be careful to place the B sites right between the nodes of the hypercubic lattice occupied by A sites (see, e.g., Ref. 17). However, the main reason to consider the particular quasi-1D case in the present work is the possibility of making contact with quasi-1D experimental systems with AB_2 unit cell, such as the compounds listed above, and recent numerical work[20] as well.

The structure of the paper is as follows: in Sec. II we build the functional-integral representation of quantum AB_2 Hubbard chains, whose associated Lagrangian free of spin degrees of freedom is analyzed in Sec. III. Further, in Sec. IV the effective strong-coupling Lagrangian in the doped regime is derived. In Sec. V the precise half-filled limit is taken, so to obtain the ferrimagnetic ground state and the associated quantum nonrelativistic nonlinear σ model. Section VI is devoted to the analysis of the several infinite-U regimes discussed above as a function of the increasing doping. At last, concluding remarks are left for Sec. VII.

II. FUNCTIONAL-INTEGRAL REPRESENTATION

We start by considering the Hubbard Hamiltonian for chains with AB_2 unit-cell topology (see Fig. 1) (Refs. 9 and 17),

$$\mathcal{H} = -\sum_{ij\alpha\beta\sigma} (t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^{\dagger} \hat{c}_{j\beta\sigma} + \text{H.c.}) + U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow}, \quad (1)$$

where $i=1,\ldots,N_c(=N/3)$ is the position of the unit cell, N_c (N) is the number of cells (sites), $\alpha,\beta=A,B_1,B_2$ denote the type of site in the unit cell, $\hat{c}_{i\alpha\sigma}$ $(\hat{c}_{i\alpha\sigma}^{\dagger})$ is the creation (annihilation) operator of electrons with spin $\sigma=(\uparrow,\downarrow)$ at site α of cell i, and $\hat{n}_{i\alpha\sigma}=\hat{c}_{i\alpha\sigma}^{\dagger}\hat{c}_{i\alpha\sigma}$ is the occupancy number operator. Electron hopping with energy $t_{ij}^{\alpha\beta}=t$ is allowed only between first-neighbor linked sites shown in Fig. 1, and double site occupancy costs a Coulombian repulsion energy $U>0$.

At this stage, a digression on some pertinent previous developments is instructive. Many treatments using functional-integral representation for fermionic models have made use of the so-called Hubbard-Stratonovich transformation.[31] In this context, the richness of open possibilities to express the local Coulomb repulsive interaction, which for the Hubbard model in a regular lattice reads $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, as combination of charge, spin, or pairing operators has caused much controversy over the years.[32] In particular, we mention the pioneering treatments of the Anderson model for dilute magnetic alloys (Kondo problem)[33] and of the Hubbard model for itinerant electron magnetism in transition metals.[34] For example, by expressing $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ in terms of charge and spin operators, with explicit spin-rotational invariance, Prange and Korenman[35] and Hubbard[36] were able to derive the Hartree-Fock saddle-point approximation for the Hubbard model, as well as an effective Heisenberg model and its associated spin-wave excitations. An important aspect of their treatment is that spin-rotational invariance is implemented through the average over local directions of the magnetization using a proper local coordinate system previously proposed in the context of a local-band theory of itinerant ferromagnetism.[37] Moreover, regarding the interaction term, it has been shown[38] that, among the identities

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{1}{2}(1-b_c)\hat{\rho}_i - \sum_{\gamma=c,x,y,z} b_\gamma (\hat{S}_i^{\gamma})^2, \quad (2)$$

where the parameters b_γ are restricted to $\Sigma_\gamma b_\gamma=2$, the spin-1/2 operators read $\hat{S}_i^{\gamma}=(1/2)\Sigma_{\sigma\sigma'}\hat{c}_{i\sigma'}^{\dagger}\hat{\sigma}_{\sigma'\sigma}^{\gamma}\hat{c}_{i\sigma}$, for $\gamma=x,y,z$, with $\hat{\sigma}^{\gamma}$ denoting the Pauli matrices $(\hbar\equiv 1)$, and $\hat{S}_{i,\sigma\sigma'}^{c}=(i/2)\delta_{\sigma\sigma'}$, two are special ones,

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{\hat{\rho}_i^2}{4} - (\hat{S}_i^z)^2 \tag{3}$$

for $b_c=b_z=1$ and $b_x=b_y=0$ (longitudinal decomposition), and

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{\hat{\rho}_i}{2} - (\hat{S}_i^x)^2 - (\hat{S}_i^y)^2 \tag{4}$$

for $b_x=b_y=1$ and $b_c=b_z=0$ (transversal decomposition). In fact, in both cases a diagrammatic perturbation theory built[38] from the functional-integral representation generates a diagrammatic structure completely equivalent to the one emulated from the standard many-body perturbation theory, i.e., there are no diagrams that violates Pauli's principle or spin conservation. This is so because in both cases the identities (3) and (4) are proved with no use of the fermion or the spin-1/2 identities $\hat{\rho}_i^2=\hat{\rho}_i$ and $(\hat{S}_i^{\pm})^2=0$, respectively. In principle, the use of the latter identities cause no harm; however, depending on the level of approximation, such as saddle point,[39] perturbation theory,[38] or RG,[40] care must be exercised in order to grasp a proper physical solution. Furthermore, if spin-rotational invariance is imperative to attain a desirable RG fixed point (e.g., Heisenberg), a combination of the two referred decompositions, treating charge and spin degrees of freedom on equal foot, allows one to properly describe the finite-T magnetic critical phenomena of the Hubbard model in $d=3$, with inclusion of both charge and spin-fluctuation effects.[40] In particular, a criterion, beyond the mean-field one, for the occurrence of a continuous ferromagnetic transition was derived[40] under the constraint of charge conservation. It is also worth mentioning a recent functional-RG approach[41] to the (symmetric) Anderson impurity model, in which the authors have implemented Hubbard-Stratonovich fields associated with transverse and longitudinal spin fluctuations. They concluded[41] that a decoupling which manifestly respects the spin-rotational invariance of the problem gives rise to the lowest quasiparticle weight.

On the other hand, much effort has been devoted to study the Hubbard model in low-dimensional systems motivated by Anderson's proposal[42] that the strong-coupling limit of the Hubbard model might help to unveil the underlying physics of the high-T_c superconductors,[25] including related phenomena, such us Mott metal-insulator transitions and exotic magnetic phases. Indeed, Schulz[43] and Weng *et al.*[44] have proposed functional approaches to study the magnetic properties of the 2D Hubbard model in the strong-coupling regime, and superconducting properties as well.[45] In these studies the authors have used decomposition shown in Eq. (3) for the interaction term, with $(\hat{S}_i^z)^2 \rightarrow (\hat{\mathbf{S}}_i\cdot\mathbf{n}_i)^2$ and a local reference frame varying in space and time with a local quantization axis defined by $\mathbf{n}_i$ at a given site i, which is connected to the static z-quantization axis of the laboratory system by a $SU(2)/U(1)$ matrix transformation, much in accord with the framework developed by Korenman and Prange[35] and Hubbard[36] to endow spin-rotational invariance. Weng *et al.*[12] also used these ideas to study the large-U 1D Hubbard model. These studies have been carried out in detail[12] and, in particular, the authors showed that, through the use of a decomposition obtained from Eq. (4) with $(\hat{S}_i^x)^2+(\hat{S}_i^y)^2 \rightarrow 2(\hat{\mathbf{S}}_i\cdot\mathbf{n}_i)^2$ and plausible physical arguments, the linearization of the interaction term can be done without explicit use of the Hubbard-Stratonovich transformation. In the following, we shall use the latter procedure to investigate the Hubbard model on the AB_2 chain. Due to the special topology of its unit cell, the ground state of this chain exhibits long-range ferrimagnetism at half filling and a variety of magnetic phases driven by doping.

We first note that the interaction term can be rewritten to explicitly incorporate the charge-density operator (electron charge $\equiv 1$), $\hat{\rho}_{i\alpha}=\hat{n}_{i\alpha\uparrow}+\hat{n}_{i\alpha\downarrow}$, and the spin degrees of freedom, expressed by the spin-1/2 operator on the AB_2 structure, $\hat{\mathbf{S}}_{i\alpha}=(1/2)\Sigma_{\sigma\sigma'}\hat{c}^{\dagger}_{i\alpha\sigma'}\hat{\sigma}_{\sigma'\sigma}\hat{c}_{i\alpha\sigma}$,

$$\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} = \frac{1}{2}\hat{\rho}_{i\alpha} - 2(\hat{\mathbf{S}}_{i\alpha}\cdot\mathbf{n}_{i\alpha})^2, \tag{5}$$

where $\mathbf{n}_{i\alpha}$ is a unit-vector field to be properly defined below. Notice that the sum over $\hat{\rho}_{i\alpha}$, implied in the substitution of Eq. (5) into Eq. (1), just gives rise to the (constant) total number of electrons. By defining an arbitrary function $W(\mathbf{n}_{i\alpha})$ normalized to unit,

$$\int d^2\mathbf{n}_{i\alpha} W(\mathbf{n}_{i\alpha}) = 1, \tag{6}$$

with specific form to be suitably chosen below, the following identity[12] concerning the interaction term in Eq. (1) applies:

$$\int \prod_{i\alpha} [d^2\mathbf{n}_{i\alpha} W(\mathbf{n}_{i\alpha})] \exp\left(\sum_{i\alpha} \hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow}\right) = \int \prod_{i\alpha} [d^2\mathbf{n}_{i\alpha} W(\mathbf{n}_{i\alpha})] \exp\left\{\sum_{i\alpha}\left[\frac{1}{2}\hat{\rho}_{i\alpha} - 2(\hat{\mathbf{S}}_{i\alpha}\cdot\mathbf{n}_{i\alpha})^2\right]\right\}, \tag{7}$$

in which Eq. (5) has been used.

The standard procedure[10,46] to calculate the partition function, $\mathcal{Z}=\mathrm{Tr}[\exp(-\beta\mathcal{H})]$, at a temperature $k_BT=\beta$, consists in slicing the continuous imaginary-time range $\tau\in[0,\beta)$ into M discrete intervals $[\tau_r,\tau_{r+1})$ of equal size $\delta\tau$, with $r=0,1,\ldots,M$, $\tau_0=0$, $\tau_M=\beta$, and $\beta=M\delta\tau$, in the limit $M\rightarrow\infty$ and $\delta\tau\rightarrow 0$. The Trotter formula allows to express $\mathcal{Z}$ as

$$\mathcal{Z} = \mathrm{Tr}\left\{\hat{T}\prod_r \exp[-\delta\tau\mathcal{H}(\tau_r)]\right\}, \tag{8}$$

where $\hat{T}$ denotes the time-ordering operator. In order to properly deal with anticommuting fermionic operators, a set of Grassmann fields, $\{c^{\dagger}_{i\alpha\sigma}(\tau_r), c_{i\alpha\sigma}(\tau_r)\}$, must be introduced, with identity for each time τ_r expressed by

$$\mathbf{1} = \int \prod_{i\alpha\sigma} [dc^{\dagger}_{i\alpha\sigma} dc_{i\alpha\sigma} e^{-c^{\dagger}_{i\alpha\sigma}c_{i\alpha\sigma}}] |\{c_{i\alpha\sigma}\}\rangle\langle\{c_{i\alpha\sigma}\}|, \tag{9}$$

where $\{|\{c_{i\alpha\sigma}\}\rangle\}$ denotes a basis of (overcomplete) fermionic coherent states in which the trace is performed. By inserting identities (7) and (9) for each time interval into Eq. (8), using the boundary conditions imposed by the trace operation,

$\mathbf{n}_{i\alpha}(0)=\mathbf{n}_{i\alpha}(\beta)$, $c^{\dagger}_{i\alpha\sigma}(0)=c^{\dagger}_{i\alpha\sigma}(\beta)$, and $c_{i\alpha\sigma}(0)=c_{i\alpha\sigma}(\beta)$, and taking the M and $\delta\tau$ limits, one obtains

$$\mathcal{Z}=\int\prod_{i\alpha}\mathcal{D}^2\mathbf{n}_{i\alpha}\prod_{i\alpha\sigma}[\mathcal{D}c^{\dagger}_{i\alpha\sigma}\mathcal{D}c_{i\alpha\sigma}]\exp\left\{-\int_0^{\beta}\mathcal{L}(\tau)d\tau\right\}, \tag{10}$$

with the measures defined as

$$\mathcal{D}^2\mathbf{n}_{i\alpha}\equiv\lim_{M\to\infty}\prod_r\{d^2\mathbf{n}_{i\alpha}(\tau_r)W[\mathbf{n}_{i\alpha}(\tau_r)]\} \tag{11}$$

and

$$\mathcal{D}c^{\dagger}_{i\alpha\sigma}\mathcal{D}c_{i\alpha\sigma}\equiv\lim_{M\to\infty}\prod_r[dc^{\dagger}_{i\alpha\sigma}(\tau_r)dc_{i\alpha\sigma}(\tau_r)]. \tag{12}$$

Above, we have also used that

$$e^{-\Sigma_{i\alpha\sigma}c^{\dagger}_{i\alpha\sigma}(\tau_r)c_{i\alpha\sigma}(\tau_r)}\langle c_{i\alpha\sigma}(\tau_{r-1})|e^{\delta\tau\Sigma_{ij\alpha\beta\sigma}(t^{\alpha\beta}_{ij}c^{\dagger}_{i\alpha\sigma}c_{j\beta\sigma}+\mathrm{H.c.})}|c_{i\alpha\sigma}(\tau_r)\rangle$$
$$=e^{\delta\tau\Sigma_{ij\alpha\beta\sigma}(t^{\alpha\beta}_{ij}c^{\dagger}_{i\alpha\sigma}c_{j\beta\sigma}+\mathrm{H.c.})}e^{-\Sigma_{i\alpha\sigma}c^{\dagger}_{i\alpha\sigma}(\tau_r)[c_{i\alpha\sigma}(\tau_r)-c_{i\alpha\sigma}(\tau_{r-1})]}, \tag{13}$$

where in the second exponential of the right-hand side the first and second terms comes, respectively, from the exponential term in Eq. (9) and the factor introduced by the time-ordered matrix element involving the coherent states $|\{c_{i\alpha\sigma}(\tau_{r-1})\}\rangle$ and $|\{c_{i\alpha\sigma}(\tau_r)\}\rangle$. In the continuous $\delta\tau\to 0$ imaginary-time limit the AB_2 Hubbard Lagrangian thus becomes

$$\mathcal{L}(\tau)=\sum_{i\alpha\sigma}c^{\dagger}_{i\alpha\sigma}\partial_{\tau}c_{i\alpha\sigma}-\sum_{ij\alpha\beta\sigma}(t^{\alpha\beta}_{ij}c^{\dagger}_{i\alpha\sigma}c_{j\beta\sigma}+\mathrm{H.c.})+U\sum_{i\alpha}\left[\frac{\rho_{i\alpha}}{2}-2(\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha})^2\right]. \tag{14}$$

Above, we have made use of the relation between the set of normally ordered creation and annihilation operators and the anticommuting Grassmann fields, $\{\hat{c}^{\dagger}_{i\alpha\sigma},\hat{c}_{i\alpha\sigma}\}\leftrightarrow\{c^{\dagger}_{i\alpha\sigma},c_{i\alpha\sigma}\}$, to formally replace operators $\hat{\rho}_{i\alpha}$ and $\hat{\mathbf{S}}_{i\alpha}$ by their respective counterparts, $\rho_{i\alpha}$ and $\mathbf{S}_{i\alpha}$, expressed in terms of Grassmann fields.

By combining Eq. (5), in the $\{c^{\dagger}_{i\alpha\sigma},c_{i\alpha\sigma}\}$ formalism, with the relation $(\rho_{i\alpha})^2=\rho_{i\alpha}+2n_{i\alpha\uparrow}n_{i\alpha\downarrow}$, we obtain $(\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha})^2=\rho_{i\alpha}(2-\rho_{i\alpha})/4$, which vanishes in the cases of double occupancy or vacancy, and equals 1/4 for single occupation of site $i\alpha$. Now, if one defines the unit field $\mathbf{n}_{i\alpha}$ to point along the (local) spin-quantization axis at site $i\alpha$, such that $\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha}=\pm 1/2$, we can consistently write that

$$\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha}=\frac{p_{i\alpha}}{2}\rho_{i\alpha}(2-\rho_{i\alpha}),\quad |p_{i\alpha}|^2=1, \tag{15}$$

where we choose the staggered local factor $p_{i\alpha}=+1$ (-1) for sites $\alpha=B_1,B_2$ (A), according to the ferrimagnetic ground state predicted by Lieb's theorem for the AB_2 Hubbard chains at half filling (see Fig. 1). Indeed, Eq. (15) can be also reinforced by the proper Gaussian choice for the function $W(\mathbf{n}_{i\alpha})$ at a certain time τ,

$$W(\mathbf{n}_{i\alpha})=\mathcal{A}\exp\left\{-\gamma\left[\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha}-\frac{p_{i\alpha}}{2}\rho_{i\alpha}(2-\rho_{i\alpha})\right]^2\right\}, \tag{16}$$

where $\mathcal{A}$ is a normalization constant and the delta-like limit $\gamma\to\infty$ is taken. As a consequence, Lagrangian (14) becomes linearized in the interaction term,

$$\mathcal{L}(\tau)=\sum_{i\alpha\sigma}c^{\dagger}_{i\alpha\sigma}\partial_{\tau}c_{i\alpha\sigma}-\sum_{ij\alpha\beta\sigma}(t^{\alpha\beta}_{ij}c^{\dagger}_{i\alpha\sigma}c_{j\beta\sigma}+\mathrm{H.c.})+U\sum_{i\alpha}\left(\frac{\rho_{i\alpha}}{2}-p_{i\alpha}\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha}\right). \tag{17}$$

It is convenient[12] to locally rotate the spin-quantization axis in order to express $\mathcal{L}$ as function of a new set of fermionic fields, whose associated spins point along the global z axis. By defining the $\mathrm{SU}(2)/U(1)$ unitary rotation matrix,

$$U_{i\alpha}=\exp\left[-\frac{i}{2}\theta_{i\alpha}\frac{(\mathbf{z}\times\mathbf{n}_{i\alpha})}{|\mathbf{z}\times\mathbf{n}_{i\alpha}|}\cdot\hat{\sigma}\right], \tag{18}$$

where $\mathbf{z}$ is the unitary vector along the z axis, or, explicitly,

$$U_{i\alpha}=\begin{bmatrix}\cos\left(\frac{\theta_{i\alpha}}{2}\right) & -\sin\left(\frac{\theta_{i\alpha}}{2}\right)e^{-i\phi_{i\alpha}}\\ \sin\left(\frac{\theta_{i\alpha}}{2}\right)e^{i\phi_{i\alpha}} & \cos\left(\frac{\theta_{i\alpha}}{2}\right)\end{bmatrix}, \tag{19}$$

acting as

$$U^{\dagger}_{i\alpha}(\hat{\sigma}\cdot\mathbf{n}_{i\alpha})U_{i\alpha}=\hat{\sigma}^z, \tag{20}$$

a new set of anticommuting fields can be obtained to transform according to

$$a_{i\alpha\sigma}=\sum_{\sigma'}(U^{\dagger}_{i\alpha})_{\sigma\sigma'}c_{i\alpha\sigma'}. \tag{21}$$

Above, $\theta_{i\alpha}$ is the polar angle between $\mathbf{n}_{i\alpha}$ and $\mathbf{z}$, and $\phi_{i\alpha}\in[0,2\pi)$ is an arbitrary azimuth angle, due to the $U(1)$ freedom of choice for $U_{i\alpha}$. We use here the notation in which, e.g., $(U_{i\alpha})_{1,2}=(U_{i\alpha})_{\uparrow\downarrow}$. These definitions, along with the choice for $p_{i\alpha}$, allow to identify the ferrimagnetic ordering of Fig. 1 with the set $\{\theta_{iA}=\theta_{iB_1}=\theta_{iB_2}=0\}$, for all i.

Substitution of Eqs. (18) and (21) into Eq. (17), along with both $\mathbf{S}_{i\alpha}\cdot\mathbf{n}_{i\alpha}=S^z_{i\alpha}$ and $\rho_{i\alpha}$ expressed in terms of $\{a^{\dagger}_{i\alpha\sigma},a_{i\alpha\sigma}\}$, leads to

$$\mathcal{L}=\mathcal{L}_0+\mathcal{L}_n, \tag{22}$$

where

$$\mathcal{L}_0(\tau)=\sum_{i\alpha\sigma}a^{\dagger}_{i\alpha\sigma}\partial_{\tau}a_{i\alpha\sigma}-\sum_{ij\alpha\beta\sigma}[t^{\alpha\beta}_{ij}a^{\dagger}_{i\alpha\sigma}a_{j\beta\sigma}+\mathrm{H.c.}]+\frac{U}{2}\sum_{i\alpha\sigma}(1-p_{i\alpha}\sigma)a^{\dagger}_{i\alpha\sigma}a_{i\alpha\sigma} \tag{23}$$

and

$$\mathcal{L}_n(\tau) = \sum_{i\alpha\sigma\sigma'} a^{\dagger}_{i\alpha\sigma'}(U^{\dagger}_{i\alpha}\partial_\tau U_{i\alpha})_{\sigma'\sigma}a_{i\alpha\sigma} - \sum_{ij\alpha\beta\sigma\sigma'} t^{\alpha\beta}_{ij}[a^{\dagger}_{i\alpha\sigma'}(U^{\dagger}_{i\alpha}U_{j\beta}-1)_{\sigma'\sigma}a_{j\beta\sigma} + \text{H.c.}]. \quad (24)$$

It is interesting to note that the spin degrees of freedom do not appear in $\mathcal{L}_0$, and are now restricted to $\mathcal{L}_n$, which includes both spin and charge dynamics intrinsically coupled.

III. ANALYSIS OF $\mathcal{H}_0$

Let us first focus on $\mathcal{L}_0$, and its associated Hamiltonian $\mathcal{H}_0$, free of the spin-related vector fields $\mathbf{n}_{i\alpha}$. After a Wick rotation,[46] the resulting $\mathcal{H}_0$ can be diagonalized in the momentum space (of first Brillouin zone $k=6\pi j/N-\pi, j=1,\ldots,N/3$, where the length of the unit cell is set to unity), by initially defining the new set of fermionic fields,

$$A_{k\sigma} = \frac{1}{2}(a_{kB_1\sigma} + a_{kB_2\sigma}) + \frac{1}{\sqrt{2}}e^{ik/2}a_{kA\sigma},$$

$$B_{k\sigma} = \frac{1}{2}(a_{kB_1\sigma} + a_{kB_2\sigma}) - \frac{1}{\sqrt{2}}e^{ik/2}a_{kA\sigma},$$

$$e_{k\sigma} = \frac{1}{\sqrt{2}}(a_{kB_1\sigma} - a_{kB_2\sigma}). \quad (25)$$

The above relations are a signature of the quasi-1D structure of the system. In particular, the phase factor $e^{ik/2}$ results directly from the AB_2 topology of the unit cell, in which the B_1 and B_2 sites are located at a distance 1/2 (in the unit of length used) ahead of the A site. In this representation we write[47]

$$\mathcal{H}_0 = \sum_{k\sigma}\varepsilon_k[A^{\dagger}_{k\sigma}A_{k\sigma} - B^{\dagger}_{k\sigma}B_{k\sigma}] + \frac{U}{2}\sum_{k\sigma}(1-\sigma)e^{\dagger}_{k\sigma}e_{k\sigma} + \frac{U}{2}\sum_{k\sigma}[A^{\dagger}_{k\sigma}A_{k\sigma} + B^{\dagger}_{k\sigma}B_{k\sigma}] - \frac{U}{2}\sum_{k\sigma}\sigma[A^{\dagger}_{k\sigma}B_{k\sigma} + B^{\dagger}_{k\sigma}A_{k\sigma}], \quad (26)$$

where

$$\varepsilon_k = -2\sqrt{2}t\cos(k/2). \quad (27)$$

The tight-binding ($U=0$) spectrum of $\mathcal{H}_0$ presents two dispersive bands plus a nondispersive flat one, related to the field operators $\{e^{\dagger}_{k\sigma}, e_{k\sigma}\}$, with macroscopic degeneracy [see Fig. 2(a)]. Clearly, this band structure is in close connection with the AB_2 unit-cell topology. Indeed, linear Hubbard chains do not present nondispersive bands but only two k-dependent modes.[10] The high degeneracy of the flat band, which maintains even for $U\neq 0$, is actually responsible for the ferrimagnetism of AB_2 Hubbard chains at $T=0$.[9] In this sense, ground-state ferrimagnetism in linear Hubbard chains is forbidden by Lieb's theorem.[8]

For $U\neq 0$ the exact diagonalization of $\mathcal{H}_0$ is possible through the Bogoliubov transformation,

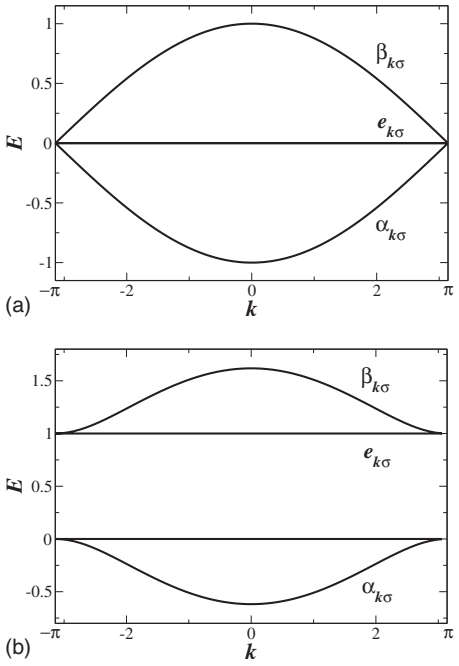

FIG. 2. Energy spectrum of the Hamiltonian (26): (a) tight-binding ($U=0$) approach (energy in units of $2\sqrt{2}t$); (b) band structure for $U=2\sqrt{2}t$ (energy in units of U). Notice that the $U=0$ spin degeneracy of the flat e bands is lift by the Coulombian coupling, so that $e_{k\uparrow}=0$ and $e_{k\downarrow}=U$, with presence of a Hubbard gap U.

$$A_{k\sigma} = u_k\alpha_{k\sigma} - \sigma v_k\beta_{k\sigma}, \quad B_{k\sigma} = \sigma v_k\alpha_{k\sigma} + u_k\beta_{k\sigma}, \quad (28)$$

subject to $(u_k)^2+(v_k)^2=1$, in order to preserve the anticommutation fermionic relations, and to a 4π periodicity of the sets $\{u_k, v_k\}$ and $\{\alpha_{k\sigma}, \beta_{k\sigma}\}$, since $A_{(k+2\pi)\sigma}=B_{k\sigma}$, due to the ferrimagnetic ground-state structure. The diagonalized $\mathcal{H}_0$ thus reads

$$H_0 = -\sum_{k\sigma}\left(E_k - \frac{U}{2}\right)\alpha^{\dagger}_{k\sigma}\alpha_{k\sigma} + \sum_{k\sigma}\left(E_k + \frac{U}{2}\right)\beta^{\dagger}_{k\sigma}\beta_{k\sigma} + \sum_{k\sigma}\frac{U}{2}(1-\sigma)e^{\dagger}_{k\sigma}e_{k\sigma}, \quad (29)$$

where

$$u_k = \frac{1}{\sqrt{2}}\left(1 + \frac{|\varepsilon_k|}{E_k}\right)^{1/2}, \quad v_k = \frac{1}{\sqrt{2}}\left(1 - \frac{|\varepsilon_k|}{E_k}\right)^{1/2} \quad (30)$$

and

$$E_k = \sqrt{\varepsilon_k^2 + U^2/4}. \quad (31)$$

Notice that the tight-biding spin degeneracy is lifted in the flat band (e), and that a Hubbard gap U separates the modes in which spins at B_1 and B_2 sites are up ($e_{k\uparrow}$; favored configuration according to the choice for $p_{i\alpha}$) and down ($e_{k\downarrow}$) [see Fig. 2(b)]. Each of these flat bands accommodate $N/3$ degenerate states. On the other hand, the dispersive bands remain spin degenerated, also with a gap U separating low (α)-energy and high (β)-energy states. Actually, the low-energy modes (α and $e_{k\uparrow}$) represent ferrimagnetic configurations with single occupancy, in which spins at sites A

(B_1, B_2) point down (up) (see Fig. 1). The energy gap to the high-energy modes (β and $e_{k\downarrow}$) is related to the energy cost U due to the presence of double occupancy. As a consequence, the properties of the strong-coupling regime below half filling become mainly driven by electrons in the lowest-energy bands.

We mention that in Ref. 9 Macêdo *et al.* have also studied the Hartree-Fock structure of the AB_2 Hubbard Hamiltonian, and their results for the half-filled strong-coupling limit are fully compatible with the band structure shown in Fig. 2(b). In particular, for $U \to \infty$, Nagaoka's mechanism (fully polarized ground state) dominates and the Hartree-Fock band structure is tight-binding-like [see Fig. 2(a)], with spin splitting $U \to \infty$.

IV. EFFECTIVE LAGRANGIAN IN THE STRONG-COUPLING LIMIT BELOW HALF FILLING

Our aim now is to obtain an effective strong-coupling Lagrangian of the AB_2 Hubbard chains in the doped regime. By expanding Eq. (30) for $U \gg t$ and defining auxiliary spinless fermionic fields[12] in direct space as

$$\alpha_i = \sqrt{\frac{3}{N}} \sum_{\sigma} \theta(\sigma) \sum_{k} e^{ikx_i} \alpha_{k\sigma},$$

$$\alpha_i^{(1/2)} = \sqrt{\frac{3}{N}} \sum_{\sigma} \theta(-\sigma) \sum_{k} e^{ikx_i} e^{-ik/2} \alpha_{k\sigma},$$

$$\beta_i = \sqrt{\frac{3}{N}} \sum_{\sigma} \theta(-\sigma) \sum_{k} e^{ikx_i} \beta_{k\sigma},$$

$$\beta_i^{(1/2)} = \sqrt{\frac{3}{N}} \sum_{\sigma} \theta(\sigma) \sum_{k} e^{ikx_i} e^{-ik/2} \beta_{k\sigma}, \tag{32}$$

where $\theta(\sigma)$ denotes the Heaviside function and the phase factor $e^{-ik/2}$ signalizes the quasi-1D AB_2 structure, we find a perturbative expression for the fields $\{A_{i\sigma}, B_{i\sigma}\}$, such that, up to order $J \equiv 4t^2/U \ll 1$ in the low-energy sector,

$$\mathcal{H}_0 = -J \sum_i [\alpha_i^\dagger \alpha_i + \alpha_i^{(1/2)\dagger} \alpha_i^{(1/2)} - \beta_i^\dagger \beta_i - \beta_i^{(1/2)\dagger} \beta_i^{(1/2)}]$$
$$+ U \sum_i [\beta_i^\dagger \beta_i + \beta_i^{(1/2)\dagger} \beta_i^{(1/2)} + e_{i\downarrow}^\dagger e_{i\downarrow}] - \frac{J}{2} \sum_i [\alpha_i^\dagger \alpha_{i+1}$$
$$+ \alpha_i^{(1/2)\dagger} \alpha_{i+1}^{(1/2)} - \beta_i^\dagger \beta_{i+1} - \beta_i^{(1/2)\dagger} \beta_{i+1}^{(1/2)} + \text{H.c.}]. \tag{33}$$

In first order, the $U \gg t$ expansion of the fields identifies $\alpha_i^{(1/2)} \approx a_{iA\downarrow}$ and $\alpha_i \approx (a_{iB_1\uparrow} + a_{iB_2\uparrow})/\sqrt{2}$, a result compatible with the low-energy spin configurations discussed in the preceding section. For the high-energy bands the situation is opposite, with spins up (down) present at sites A (B_1, B_2) with double occupation. Also, notice from Eq. (33) that J defines the width of the bands in the strong-coupling limit, whereas the gap between the low- and high-energy bands remains essentially determined by U.

Below half filling, one has to additionally exclude from $\mathcal{H}_0$ the energy terms containing only field operators related to the high-energy bands $(\beta_i, \beta_i^{(1/2)}, e_{i\downarrow})$. In this regime, the Lagrangian associated with $\mathcal{H}_0$ in the low-energy sector thus reads, up to order J,

$$\mathcal{L}_0 = \sum_i \alpha_i^\dagger \partial_\tau \alpha_i - J \sum_i [\alpha_i^\dagger \alpha_i + \alpha_i^{(1/2)\dagger} \alpha_i^{(1/2)}]$$
$$- \frac{J}{2} \sum_i [\alpha_i^\dagger \alpha_{i+1} + \alpha_i^{(1/2)\dagger} \alpha_{i+1}^{(1/2)} + \text{H.c.}]. \tag{34}$$

We now turn to the $U \gg t$ perturbative expansion of $\mathcal{L}_n$, Eq. (24). It is convenient to introduce rotation matrices either symmetric or antisymmetric with respect to the exchange operation $B_1 \leftrightarrow B_2$, such as

$$U_i^{(b)} = U_{iA}, \quad U_i^{(d)} = \frac{1}{\sqrt{2}}(U_{iB_1} + U_{iB_2}), \quad U_i^{(e)} = \frac{1}{\sqrt{2}}(U_{iB_1} - U_{iB_2}). \tag{35}$$

By performing changes in field sets as above, and expanding up to order J, we obtain

$$\mathcal{L}_n(\tau) = \mathcal{L}_n^{(1)} + \mathcal{L}_n^{(2)} + \mathcal{L}_n^{(3)} + \mathcal{L}_n^{(4)} + \mathcal{L}_n^{(5)} + \mathcal{L}_n^{(6)} + \mathcal{L}_n^{(7)} + \mathcal{L}_n^{(8)} + \mathcal{L}_n^{(9)}, \tag{36}$$

where

$$\mathcal{L}_n^{(1)} = \sum_{i\sigma\sigma'} (U_i^{(b)\dagger} \partial_\tau U_i^{(b)})_{\sigma\sigma'} \Big\{ \theta(-\sigma) \delta_{\sigma'\sigma} \alpha_i^{(1/2)\dagger} \alpha_i^{(1/2)}$$
$$+ \sqrt{2} \frac{t}{U} \delta_{\sigma',-\sigma} [\theta(-\sigma) \alpha_i^{(1/2)\dagger} (\alpha_i + \alpha_{i-1})$$
$$+ \theta(\sigma) (\alpha_i^\dagger + \alpha_{i-1}^\dagger) \alpha_i^{(1/2)}] \Big\},$$

$$\mathcal{L}_n^{(2)} = \sum_{i\sigma\sigma';\nu=d,e} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu)})_{\sigma\sigma'} \Big\{ \theta(\sigma) \frac{\delta_{\sigma'\sigma}}{2} \alpha_i^\dagger \alpha_i$$
$$+ \frac{t}{\sqrt{2}U} \delta_{\sigma',-\sigma} [\theta(\sigma) \alpha_i^\dagger (\alpha_i^{(1/2)} + \alpha_{i+1}^{(1/2)})$$
$$+ \theta(-\sigma) (\alpha_i^{(1/2)\dagger} + \alpha_{i+1}^{(1/2)\dagger}) \alpha_i] \Big\},$$

$$\mathcal{L}_n^{(3)} = \sum_{i\sigma;\nu=d,e} \frac{\theta(\sigma)}{2} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu)})_{\sigma\sigma} e_{i\uparrow}^\dagger e_{i\uparrow},$$

$$\mathcal{L}_n^{(4)} = \sum_{i\sigma\sigma';\nu,\nu'=d,e;\nu\neq\nu'} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu')})_{\sigma\sigma'} \Big\{ \frac{\theta(\sigma)}{2} \delta_{\sigma'\sigma} \alpha_i^\dagger e_{i\uparrow}$$
$$+ \frac{t}{\sqrt{2}U} \theta(-\sigma) \delta_{\sigma',-\sigma} (\alpha_i^{(1/2)\dagger} + \alpha_{i+1}^{(1/2)\dagger}) e_{i\uparrow} \Big\},$$

$$\mathcal{L}_n^{(5)} = [\mathcal{L}_n^{(4)}]^\dagger,$$

$$\mathcal{L}_n^{(6)} = -\sum_{i\sigma\sigma'} (U_i^{(b)\dagger} U_i^{(d)} - \sqrt{2})_{\sigma\sigma'} \Big\{ t\delta_{\sigma'\sigma}[\theta(-\sigma)\alpha_i^{(1/2)\dagger}\beta_i - \theta(\sigma)\beta_i^{(1/2)\dagger}\alpha_i] + t\theta(-\sigma)\delta_{\sigma',-\sigma}\alpha_i^{(1/2)\dagger}\alpha_i + \sqrt{2}\frac{t^2}{U}\delta_{\sigma'\sigma}[\theta(-\sigma)\alpha_i^{(1/2)\dagger}(\alpha_i^{(1/2)} + \alpha_{i+1}^{(1/2)}) + \theta(\sigma)(\alpha_i^\dagger + \alpha_{i-1}^\dagger)\alpha_i] + \text{H.c.} \Big\},$$

$$\mathcal{L}_n^{(7)} = -\sum_{i\sigma\sigma'} (U_i^{(b)\dagger} U_i^{(e)})_{\sigma\sigma'} \Big\{ t\theta(-\sigma)\delta_{\sigma',-\sigma}\alpha_i^{(1/2)\dagger} e_{i\uparrow} + t\delta_{\sigma'\sigma}[\theta(-\sigma)\alpha_i^{(1/2)\dagger} e_{i\downarrow} - \theta(\sigma)\beta_i^{(1/2)\dagger} e_{i\uparrow}] + \sqrt{2}\frac{t^2}{U}\delta_{\sigma'\sigma}\theta(\sigma)(\alpha_i^\dagger + \alpha_{i-1}^\dagger)e_{i\uparrow} + \text{H.c.} \Big\},$$

$$\mathcal{L}_n^{(8)} = -\sum_{i\sigma\sigma'} (U_i^{(d)\dagger} U_{i+1}^{(b)} - \sqrt{2})_{\sigma\sigma'} \Big\{ t\delta_{\sigma'\sigma}[\theta(-\sigma)\beta_i^\dagger \alpha_{i+1}^{(1/2)} - \theta(\sigma)\alpha_i^\dagger \beta_{i+1}^{(1/2)}] + t\theta(\sigma)\delta_{\sigma',-\sigma}\alpha_i^\dagger \alpha_{i+1}^{(1/2)} + \sqrt{2}\frac{t^2}{U}\delta_{\sigma'\sigma}[\theta(\sigma)\alpha_i^\dagger(\alpha_i + \alpha_{i+1}) + \theta(-\sigma)(\alpha_i^{(1/2)\dagger} + \alpha_{i+1}^{(1/2)\dagger})\alpha_{i+1}^{(1/2)}] + \text{H.c.} \Big\},$$

$$\mathcal{L}_n^{(9)} = -\sum_{i\sigma\sigma'} (U_i^{(e)\dagger} U_{i+1}^{(b)})_{\sigma\sigma'} \Big\{ t\theta(\sigma)\delta_{\sigma',-\sigma} e_{i\uparrow}^\dagger \alpha_{i+1}^{(1/2)} + t\delta_{\sigma'\sigma}[\theta(-\sigma)e_{i\downarrow}^\dagger \alpha_{i+1}^{(1/2)} - \theta(\sigma)e_{i\uparrow}^\dagger \beta_{i+1}^{(1/2)}] + \sqrt{2}\frac{t^2}{U}\delta_{\sigma'\sigma}\theta(\sigma)e_{i\uparrow}^\dagger(\alpha_i + \alpha_{i+1}) + \text{H.c.} \Big\}.$$

Above, terms containing exclusively fields related to the high-energy bands have already been excluded in the regime below half filling. Notice, however, that hopping between low- and high-energy bands is still present in $\mathcal{L}_n$ (for instance, $e_{i\downarrow}^\dagger \alpha_{i+1}^{(1/2)}$ in $\mathcal{L}_n^{(9)}$). Such terms must be treated in a perturbative analysis as follows.

First, let $|\Phi_0(N)\rangle$ be the unperturbed ferrimagnetic state at half-filled band, with $N_e = N$ electrons filling completely the low-energy modes $(\alpha, e_{i\uparrow})$, empty high-energy states $(\beta, e_{i\downarrow})$, and energy $E_0(N)$. In the context of a second-order Rayleigh-Schrödinger perturbative theory consistent with the strong-coupling expansions up to t^2/U, the virtual perturbative states $|\gamma_k, \sigma\rangle$ contain $N-1$ electrons in the low-energy bands and one electron with spin σ promoted to a high-energy band, either β [with energy $E_k^\gamma = E_0(N-1) + E_k + U/2$] or $e_{i\downarrow}$ [with $E_k^\gamma = E_0(N-1) + U$]. Contributions to the perturbative Hamiltonian $\mathcal{H}_1$ thus come from all terms in Eq. (36) involving crossed field products that represent transitions from a low-energy to a high-energy band or vice versa. In second order of perturbation, the energy of the perturbed state is $E = E_0(N) + \Delta E$, where

$$\Delta E = \langle \Phi_0 | H_1 | \Phi_0 \rangle + \sum_{k\sigma} \frac{\langle \Phi_0 | H_1 | \gamma_k, \sigma \rangle \langle \gamma_k, \sigma | H_1 | \Phi_0 \rangle}{E_0 - E_k^\gamma}. \tag{37}$$

The explicit calculation allows to write $\Delta E = \langle \Phi_0 | \mathcal{H}' | \Phi_0 \rangle$, with the effective Hamiltonian $\mathcal{H}'$ playing the same role as $\mathcal{H}_1$ in the regime below half filling and up to order t^2/U.

In the sequence, the Lagrangian associated with $\mathcal{H}'$ can be finally obtained, which, summed up with $\mathcal{L}_0$, Eq. (34), gives rise to the effective low-lying Lagrangian of the Hubbard AB_2 chains in the strong-coupling limit (up to order t^2/U),

$$\mathcal{L}_{eff}(\tau) = \mathcal{L}^{(I)} + \mathcal{L}^{(II)} + \mathcal{L}^{(III)} + \mathcal{L}^{(IV)} + \mathcal{L}^{(V)}, \tag{38}$$

where

$$\mathcal{L}^{(I)} = \sum_i \alpha_i^\dagger \partial_\tau \alpha_i + \sum_i \alpha_i^{(1/2)\dagger} \partial_\tau \alpha_i^{(1/2)} + \sum_i e_{i\uparrow}^\dagger \partial_\tau e_{i\uparrow},$$

$$\mathcal{L}^{(II)} = \sum_{i\sigma} \Big\{ \theta(-\sigma)(U_i^{(b)\dagger}\partial_\tau U_i^{(b)})_{\sigma\sigma}\alpha_i^{(1/2)\dagger}\alpha_i^{(1/2)} + \theta(\sigma)\frac{1}{2}[(U_i^{(d)\dagger}\partial_\tau U_i^{(d)})_{\sigma\sigma} + (U_i^{(e)\dagger}\partial_\tau U_i^{(e)})_{\sigma\sigma}] \times (\alpha_i^\dagger \alpha_i + e_{i\uparrow}^\dagger e_{i\uparrow}) + \Big[\theta(\sigma)\frac{1}{2}[(U_i^{(d)\dagger}\partial_\tau U_i^{(e)})_{\sigma\sigma} + (U_i^{(e)\dagger}\partial_\tau U_i^{(d)})_{\sigma\sigma}]\alpha_i^\dagger e_{i\uparrow} + \text{H.c.} \Big] \Big\},$$

$$\mathcal{L}^{(III)} = -t\sum_{i\sigma} \{ \theta(-\sigma)(U_i^{(b)\dagger}U_i^{(d)})_{\sigma,-\sigma}\alpha_i^{(1/2)\dagger}\alpha_i + \theta(\sigma)(U_i^{(d)\dagger}U_{i+1}^{(b)})_{\sigma,-\sigma}\alpha_i^\dagger \alpha_{i+1}^{(1/2)} + \theta(-\sigma)(U_i^{(b)\dagger}U_i^{(e)})_{\sigma,-\sigma}\alpha_i^{(1/2)\dagger}e_{i\uparrow} + \theta(\sigma)(U_i^{(e)\dagger}U_{i+1}^{(b)})_{\sigma,-\sigma}e_{i\uparrow}^\dagger \alpha_{i+1}^{(1/2)} + \text{H.c.} \},$$

$$\mathcal{L}^{(IV)} = -\frac{J}{4}\sum_{i;i'=i,i+1;\sigma} \{ \theta(\sigma)|(U_i^{(d)\dagger}U_{i'}^{(b)})_{\sigma\sigma}|^2 \alpha_i^\dagger \alpha_i + \theta(-\sigma)|(U_i^{(b)\dagger}U_{i'}^{(d)})_{\sigma\sigma}|^2 \alpha_i^{(1/2)\dagger}\alpha_i^{(1/2)} \} - \frac{J}{4}\sum_{i;i'=i,i-1;\sigma} \{ \theta(\sigma)|(U_i^{(e)\dagger}U_{i'}^{(b)})_{\sigma\sigma}|^2 e_{i\uparrow}^\dagger e_{i\uparrow} + \theta(-\sigma)|(U_i^{(b)\dagger}U_{i'}^{(e)})_{\sigma\sigma}|^2 \alpha_i^{(1/2)\dagger}\alpha_i^{(1/2)} \},$$

$$\mathcal{L}^{(V)} = -\frac{J}{4}\sum_{i;\nu=d,e;\sigma} \{ \theta(-\sigma) \times (U_i^{(b)\dagger}U_i^{(\nu)})_{\sigma\sigma}(U_i^{(\nu)\dagger}U_{i+1}^{(b)})_{\sigma\sigma}\alpha_i^{(1/2)\dagger}\alpha_{i+1}^{(1/2)} + \text{H.c.} \} - \frac{J}{4}\sum_{i;i'=i,i+1;\sigma} \{ \theta(\sigma)(U_i^{(d)\dagger}U_{i'}^{(b)})_{\sigma\sigma}(U_{i'}^{(b)\dagger}U_i^{(e)})_{\sigma\sigma}\alpha_i^\dagger e_{i\uparrow} + \text{H.c.} \} - \frac{J}{4}\sum_{i\sigma} \{ \theta(\sigma)(U_i^{(d)\dagger}U_{i+1}^{(b)})_{\sigma\sigma}(U_{i+1}^{(b)\dagger}U_{i+1}^{(e)})_{\sigma\sigma}\alpha_i^\dagger e_{i+1\uparrow}$$

$$+\theta(\sigma)(U_i^{(d)\dagger}U_{i+1}^{(b)})_{\sigma\sigma}(U_{i+1}^{(b)\dagger}U_{i+1}^{(d)})_{\sigma\sigma}\alpha_i^\dagger\alpha_{i+1}$$
$$+\theta(\sigma)(U_i^{(e)\dagger}U_{i+1}^{(b)})_{\sigma\sigma}(U_{i+1}^{(b)\dagger}U_{i+1}^{(e)})_{\sigma\sigma}e_{i\uparrow}^\dagger e_{i+1\uparrow}$$
$$+\theta(\sigma)(U_i^{(e)\dagger}U_{i+1}^{(b)})_{\sigma\sigma}(U_{i+1}^{(b)\dagger}U_{i+1}^{(d)})_{\sigma\sigma}e_{i\uparrow}^\dagger\alpha_{i+1}+\text{H.c.}\}.$$

Above, $\mathcal{L}^{(I)}$ represents the kinetic term related to the charge degrees of freedom, whereas the kinetics of the spin degrees of freedom is described by $\mathcal{L}^{(II)}$, with a coupling to the charge fields. On the other hand, $\mathcal{L}^{(III)}$ and $\mathcal{L}^{(IV)}$ denote hopping between first neighbors for the coupled charge and spin degrees of freedom, respectively, and $\mathcal{L}^{(V)}$ represents second-neighbor hops.

From the field expansions above, the next term of order $J/t=4t/U\ll J$ in $\mathcal{L}_{eff}$ reads

$$\mathcal{L}^{(VI)}=\frac{J}{2\sqrt{2}t}\sum_{i;i'=i,i-1;\sigma}\{\theta(-\sigma)(U_i^{(b)\dagger}\partial_\tau U_i^{(b)})_{\sigma,-\sigma}\alpha_i^{(1/2)\dagger}\alpha_{i'}$$
$$+\text{H.c.}\}+\frac{J}{4\sqrt{2}t}\sum_{i;i'=i,i+1;\sigma;\nu=d,e}\{\theta(\sigma)$$
$$\times(U_i^{(\nu)\dagger}\partial_\tau U_i^{(\nu)})_{\sigma,-\sigma}\alpha_i^\dagger\alpha_{i'}^{(1/2)}+\text{H.c.}\}$$
$$+\frac{J}{4\sqrt{2}t}\sum_{i;i'=i,i+1;\sigma;\nu,\nu'=d,e;\nu\neq\nu'}\{\theta(-\sigma)$$
$$\times(U_i^{(\nu)\dagger}\partial_\tau U_i^{(\nu')})_{\sigma,-\sigma}\alpha_{i'}^{(1/2)\dagger}e_{i\uparrow}+\text{H.c.}\},\quad(39)$$

which contributes to the quantum spin dynamics and hopping in higher order.

V. HALF-FILLING LIMIT OF $\mathcal{L}_{eff}$

Precisely at half filling ($\delta=0$), the full occupation of the lower-energy bands implies $\langle\alpha_i^\dagger\alpha_i\rangle=1$, $\langle\alpha_i^{(1/2)\dagger}\alpha_i^{(1/2)}\rangle=1$, and $\langle e_{i\uparrow}^\dagger e_{i\uparrow}\rangle=1$. As a consequence, a ferrimagnetic configuration of localized electrons emerges, such that $\langle\alpha_i^\dagger\partial_\tau\alpha_i\rangle=\langle\alpha_i^{(1/2)\dagger}\partial_\tau\alpha_i^{(1/2)}\rangle=\langle e_{i\uparrow}^\dagger\partial_\tau e_{i\uparrow}\rangle=0$, with forbidden hopping [terms $\mathcal{L}^{(III)}$ and $\mathcal{L}^{(V)}$ in Eq. (38)]. The resulting effective strong-coupling Lagrangian at half filling becomes

$$\mathcal{L}_{eff}^{hf}=\sum_{i\alpha\sigma}\theta(p_{i\alpha}\sigma)(U_{i\alpha}^\dagger\partial_\tau U_{i\alpha})_{\sigma\sigma}$$
$$-\frac{J}{4}\sum_{\langle i\alpha,j\beta\rangle}\sum_\sigma\theta(p_{i\alpha}\sigma)|(U_{i\alpha}^\dagger U_{j\beta})_{\sigma\sigma}|^2,\quad(40)$$

where $\langle\cdots\rangle$ means sum over nearest neighbors. In terms of Pauli matrices, it is possible to write, according to Eq. (19),

$$U_{i\alpha}=\cos\left(\frac{\theta_{i\alpha}}{2}\right)1-i\sin\left(\frac{\theta_{i\alpha}}{2}\frac{\mathbf{z}\times\mathbf{n}_{i\alpha}}{|\mathbf{z}\times\mathbf{n}_{i\alpha}|}\right)\cdot\hat{\sigma},\quad(41)$$

such that, by defining $\mathbf{z}\wedge\mathbf{n}_{i\alpha}\equiv(\mathbf{z}\times\mathbf{n}_{i\alpha})/|\mathbf{z}\times\mathbf{n}_{i\alpha}|$,

$$\partial_\tau U_{i\alpha}=-\frac{1}{2}\sin\left(\frac{\theta_{i\alpha}}{2}\right)\partial_\tau\theta_{i\alpha}-\frac{i}{2}\cos\left(\frac{\theta_{i\alpha}}{2}\right)(\partial_\tau\theta_{i\alpha})\hat{\sigma}\cdot\frac{(\mathbf{z}\wedge\mathbf{n}_{i\alpha})}{\sin\theta_{i\alpha}}$$
$$-i\sin\left(\frac{\theta_{i\alpha}}{2}\right)\hat{\sigma}\cdot\left[\mathbf{z}\wedge\partial_\tau\left(\frac{\mathbf{n}_{i\alpha}}{\sin\theta_{i\alpha}}\right)\right].\quad(42)$$

Thus, the first matrix product in Eq. (40) is given by

$$U_{i\alpha}^\dagger\partial_\tau U_{i\alpha}=\frac{i}{2}\frac{(1-\cos\theta_{i\alpha})}{(\sin\theta_{i\alpha})^2}(\mathbf{z}\wedge\mathbf{n}_{i\alpha})\cdot(\partial_\tau\mathbf{n}_{i\alpha})\hat{\sigma}^z$$
$$-\frac{i}{2}\frac{\partial_\tau\theta_{i\alpha}}{\sin\theta_{i\alpha}}\hat{\sigma}\cdot(\mathbf{z}\wedge\mathbf{n}_{i\alpha})$$
$$-\frac{i}{2}\sin\theta_{i\alpha}\hat{\sigma}\cdot\left[\mathbf{z}\wedge\partial_\tau\left(\frac{\mathbf{n}_{i\alpha}}{\sin\theta_{i\alpha}}\right)\right],\quad(43)$$

with diagonal elements

$$(U_{i\alpha}^\dagger\partial_\tau U_{i\alpha})_{\sigma\sigma}=\frac{i}{2}\sigma\mathbf{A}(\mathbf{n}_{i\alpha})\cdot\partial_\tau\mathbf{n}_{i\alpha},\quad(44)$$

where

$$\mathbf{A}(\mathbf{n}_{i\alpha})=\frac{(1-\cos\theta_{i\alpha})}{\sin\theta_{i\alpha}}\mathbf{z}\wedge\mathbf{n}_{i\alpha}.\quad(45)$$

It is interesting to note that $\mathbf{A}$ is analogous to the magnetic vector potential of a Dirac's string placed at the $z<0$ axis.[10] In addition, a similar treatment leads to

$$|(U_{i\alpha}^\dagger U_{j\beta})_{\sigma\sigma}|^2=\frac{1+\mathbf{n}_{i\alpha}\cdot\mathbf{n}_{j\beta}}{2}.\quad(46)$$

Substituting the above results into Eq. (40), and using[12] that $\nabla_{i\alpha}\times\mathbf{A}=\mathbf{n}_{i\alpha}$, we obtain the following low-lying effective action in the strong-coupling half-filling regime:

$$S_{eff}^{hf}=S_{exc}+\sum_{i\alpha}p_{i\alpha}S_{WZ}(\mathbf{n}_{i\alpha}),\quad(47)$$

with omission of an irrelevant additive constant, in which

$$S_{exc}=-\frac{J}{8}\sum_i\sum_{\alpha=B,C}\int_0^{\beta\hbar}[\mathbf{n}_{iA}\cdot(\mathbf{n}_{i\alpha}+\mathbf{n}_{i-1\alpha})$$
$$+\mathbf{n}_{i\alpha}\cdot(\mathbf{n}_{iA}+\mathbf{n}_{i+1A})]\quad(48)$$

and

$$S_{WZ}(\mathbf{n}_{i\alpha})=-\frac{i\hbar}{2}\int_0^1 d\gamma\int_0^{\beta\hbar}d\tau\mathbf{n}_{i\alpha}\cdot(\partial_\tau\mathbf{n}_{i\alpha}\times\partial_\gamma\mathbf{n}_{i\alpha}),\quad(49)$$

where $\mathbf{n}_{i\alpha}(0,\gamma)=\mathbf{n}_{i\alpha}(\beta,\gamma)$, $\mathbf{n}_{i\alpha}(\tau,0)\equiv\mathbf{z}$, and $\mathbf{n}_{i\alpha}(\tau,1)\equiv\mathbf{n}_{i\alpha}(\tau)$. We note in Eq. (49) that $S_{WZ}(\mathbf{n}_{i\alpha})$ is proportional to the area swept by the trajectory of the quantum-fluctuating spin-related vector field $\mathbf{n}_{i\alpha}$ on a unit sphere, i.e., $\mathbf{n}_{i\alpha}(t,\gamma)$ is a smooth parametrization of the spherical cap delimited by such quantum path, satisfying the mentioned boundary conditions.[10,17]

Equations (47)–(49) are fully equivalent to the effective action obtained in Ref. 17 in a spin-based coherent-state representation[10] of the quantum AB_2 ferrimagnetic Heisenberg model of localized spins, which represents the strong-coupling limit of the AB_2 Hubbard chain at half filling. The localized character of the charge degrees of freedom in the AB_2 unit-cell structure is presented in the exchange term, Eq. (48), with the spin degrees coupled through $J=4t^2/U>0$, consistently with the ferrimagnetic ground-state configuration, in agreement with both numerical[9,13] and analytical[17] studies.

On the other hand, the Wess-Zumino action, Eq. (49), is a Berry's phaselike term,[10] and also carries relevant information on the unit-cell AB_2 topology. Indeed, one possible representation[17] consists in breaking up $\Sigma_{i\alpha} p_{i\alpha} S_{WZ}$ in Eq. (47) into antiferromagneticlike and ferromagneticlike contributions, with the latter related only to B_1 and B_2 sites. As S_{WZ} in Eq. (49) changes sign upon spin inversion ($\mathbf{n}_{i\alpha} \rightarrow -\mathbf{n}_{i\alpha}$), nearest-neighbor opposite spins in the antiferromagneticlike counterpart can be treated as follows. By separating $\mathbf{n}_{i\alpha}$ into slowly varying order-parameter ($\mathbf{m}_{i\alpha}$) and rapidly fluctuating ($\mathbf{f}_{i\alpha}$) fields, and taking the continuous space limit along with $\mathbf{n}' - \mathbf{n} \approx \partial_x \mathbf{n}$, where $\mathbf{n}'$ and $\mathbf{n}$ represent nearest-neighbor spins, the antiferromagneticlike Wess-Zumino contribution becomes proportional to the so-called Potryagin index or winding number,[10]

$$\mathcal{Q} = \frac{1}{4\pi} \int dx d\tau \mathbf{m} \cdot (\partial_\tau \mathbf{m} \times \partial_x \mathbf{m}). \tag{50}$$

On the other hand, the ferromagneticlike counterpart is related[10,17] to the spin-wave modes[14] with quadratic low-energy dispersion relation ($\sim k^z$, with dynamical exponent $z=2$). This result is strictly connected with the fact that for each Wess-Zumino term of sites A one has two similar contributions from sites B_1 and B_2. By further integrating over $\{\mathbf{f}_{i\alpha}\}$, the effective action S_{eff}^{hf} is shown[17] to be mapped onto a nonrelativistic ($z=2$) nonlinear σ model. In contrast, antiferromagnetic linear systems in $d>1$ map onto the relativistic nonlinear σ model, with linear dispersion relation ($z=1$).[10,12]

VI. DOPED REGIME IN THE INFINITE-U LIMIT

In the infinite-U limit ($J=0$) below half filling, Eq. (38) reduces to $\mathcal{L}_{eff}(\tau) = \mathcal{L}^{(I)} + \mathcal{L}^{(II)} + \mathcal{L}^{(III)}$. This means that, in such extreme condition, the hopping energy contribution is restricted to $\mathcal{L}^{(III)}$ and double occupancy is completely excluded.

A. Nagaoka state

We start with the doped regime close to half filling. In order to analyze the role of the hopping mechanism, we need to explicit the matrix products in $\mathcal{L}^{(III)}$. From Eqs. (19) and (35),

$$\frac{U_i^{(b)\dagger} U_{i'}^{(d)}}{\sqrt{2}} = \begin{pmatrix} \cos\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\cos\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) & \sin\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\cos\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) \\ -\sin\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\cos\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) & \cos\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\cos\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) \end{pmatrix}$$

and

$$\frac{U_i^{(b)\dagger} U_{i'}^{(e)}}{\sqrt{2}} = \begin{pmatrix} \sin\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\sin\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) & \cos\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\sin\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) \\ -\cos\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\sin\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) & \sin\left(\frac{\theta_{iA}}{2} - \sum_\alpha \frac{\theta_{i'\alpha}}{4}\right)\sin\left(\frac{\theta_{i'B_1} - \theta_{i'B_2}}{4}\right) \end{pmatrix},$$

where Σ_α denotes sum over $\alpha = B_1, B_2$.

By assuming a ferrimagnetic ground state, with $\{\theta_{iA} = \theta_{iB_1} = \theta_{iB_2}\}$ for all i, the off-diagonal elements in both matrix products above vanish, implying in zero hopping energy, as expected. This result is similar to the mechanism that localizes electrons precisely at half filling for any $U>0$ (Lieb's theorem).

Nevertheless, this is not the lowest-energy state of the system in the infinite-U limit *near* half filling. To attest this, we note that contributions to the hopping amplitudes come from the matrix elements $(U_i^{\dagger(d)} U_{i'}^{(b)})_{\uparrow\downarrow}$, $(U_i^{\dagger(b)} U_{i'}^{(d)})_{\downarrow\uparrow}$, $(U_i^{\dagger(e)} U_{i'}^{(b)})_{\uparrow\downarrow}$, and $(U_i^{\dagger(b)} U_{i'}^{(e)})_{\downarrow\uparrow}$, whose sum does not depend on θ_{iB_2} and is maximized for $\{\theta_{iA}=0; \theta_{iB_1}=\pi\}$. Let us first analyze the case $\{\theta_{iA}=0; \theta_{iB_1}=\theta_{iB_2}=\pi\}$ in the presence of one hole at half filling. This solution represents a fully polarized ferromagnetic (Nagaoka) state, in which the single hole behaves like a spinless fermion, free to move in the AB_2 chain structure with forbidden double occupancy. In this case one has that $|(U_i^{(b)\dagger} U_{i'}^{(d)})_{\sigma,-\sigma}| = \sqrt{2}$ and $|(U_i^{(b)\dagger} U_{i'}^{(e)})_{\sigma,-\sigma}| = 0$, thus indicating [see $\mathcal{L}^{(III)}$] that this hole itinerancy is related to hopping in the lower-energy dispersive α band; indeed, hopping from or to the higher-energy flat e band does not contribute in this regime. The Nagaoka state in the AB_2 topology has been also observed through several numerical methods.[9,13,20,21] In particular, exact-diagonalization and DMRG results have shown[20] that this metallic phase is actually characterized by the presence of holes in the low-energy dispersive band, in agreement with our results.

Substitution of the matrix elements of the Nagaoka phase leads to the effective associated Hamiltonian,

$$\mathcal{H}_{FM} = -t\sqrt{2} \sum_i \hat{P}_G [\alpha_i^\dagger (\alpha_i^{(1/2)} + \alpha_{i+1}^{(1/2)}) + \text{H.c.}] \hat{P}_G, \tag{51}$$

where the Gutzwiller projection operator, $\hat{P}_G = \Pi_{j\alpha}(1 - \hat{n}_{j\alpha\uparrow}\hat{n}_{j\alpha\downarrow})$, prevents double occupancy. Considering now N_h

holes in the AB_2 chain, the total energy calculated from $\mathcal{H}_{FM}$ is found to be

$$E = -\frac{4\sqrt{2}t}{\pi} N_c \sin\left(\frac{k_F}{2}\right), \tag{52}$$

with Fermi momentum $k_F = \pi N_h / N_c$, in agreement with Ref. 20. As a consequence, Nagaoka state's energy with a single hole at half filling moving in the α band is shown to be lower than those corresponding to the cases $\{\theta_{iA}=0; \theta_{iB_1}=\pi; \theta_{iB_2} \neq \pi\}$, in which the hole is either allowed to displace freely along the chain formed by sites A and B_1, or to remain localized at a B_2 site.

B. Phase separation and RVB states at $\delta = 1/3$

As numerical results indicate,[9,20] for doping $0.225 \lesssim \delta < 1/3$ a phase separation into coexisting metallic and insulating regions takes place in the infinite-U limit. In this case, the energy balance can turn in favor of localized states, with both spin and charge gaps, and solutions with $|(U_i^{(b)\dagger} U_{i'}^{(e)})_{\sigma,-\sigma}| \neq 0$ may arise. In particular, at commensurate doping $\delta = 1/3$ (two electrons per unit cell) the ground state is a Mott-insulating short-ranged RVB state, with spin-spin correlation length of order of the unit cell's size (exponentially decaying with distance[27]) and energy $E_{\mathrm{RVB}} \approx -2.021t$ roughly independent of the system length. Within each unit cell the pair of spins constitutes rotationally invariant singlet states.

In the context of the Wess-Zumino action arising from $\mathcal{L}^{(II)}$ (see Sec. V), it is possible to express this contribution in terms of the occupancy number fields $n_{i\alpha}$, with $\alpha = A, B_1, B_2$,

$$\mathcal{L}^{(II)} = \sum_i \{(U_{iA}^\dagger \partial_\tau U_{iA})_{\downarrow\downarrow} n_{iA} + (U_{iB_1}^\dagger \partial_\tau U_{iB_1})_{\uparrow\uparrow} n_{iB_1} + (U_{iB_2}^\dagger \partial_\tau U_{iB_2})_{\uparrow\uparrow} n_{iB_2}\}. \tag{53}$$

Possible singlet states at $\delta = 1/3$ are such that $\{n_{i'A}=1, n_{iB_1}=1, n_{iB_2}=0\}$, or $\{n_{i'A}=1, n_{iB_1}=0, n_{iB_2}=1\}$, or $\{n_{i'A}=0, n_{iB_1}=1, n_{iB_2}=1\}$, with i and i' representing either the same cell ($i'=i$) or nearest-neighbor cells ($i'=i+1$). By enumerating all singlet combinations, we first obtain the mean numbers of electrons per site: $\langle n_{iA}\rangle = 0.5$ and $\langle n_{iB_1}\rangle = \langle n_{iB_2}\rangle = 0.75$ (whose sum equals 2, as expected), in agreement with DMRG results.[20] As the rotational symmetry of singlet states requires antiparallel spins within the unit cell, an antiferromagnetic background is locally set, so that, according with results of Sec. V,

$$\mathcal{L}^{(II)} = \sum_i \frac{i}{2}\{-[\mathbf{A}(\mathbf{n}_{iA}) \cdot \partial_\tau \mathbf{n}_{iA}] n_{iA} + [\mathbf{A}(\mathbf{n}_{iB_1}) \cdot \partial_\tau \mathbf{n}_{iB_1}] n_{iB_1} + [\mathbf{A}(\mathbf{n}_{iB_2}) \cdot \partial_\tau \mathbf{n}_{iB_2}] n_{iB_2}\}. \tag{54}$$

Therefore, only the antiferromagneticlike Wess-Zumino term contributes [note that in the case of a singlet state involving a pair of spins at B_1 and B_2 sites of the same cell, we should additionally rotate, e.g., $\mathbf{n}_{iB_2} \to -\mathbf{n}_{iB_2}$, so to change the sign of its Wess-Zumino action in Eq. (49)]. Indeed, the ferromagneticlike counterpart vanishes at $\delta = 1/3$. We observe that the scheme that has led to Eq. (50) (winding number) does not apply in this case since the space derivative breaks down in unit cells with spin singlets at B_1 and B_2 sites. As a consequence, the long-range order cannot sustain and, as the spin-correlation length becomes of order of the unit cell's size, the system exhibits short-range RVB states.[10,25,26]

When considered together in an energy-minimization procedure,[20] the competition between the (metallic) Nagaoka [Eq. (52)] and (insulating) RVB (E_{RVB}) mechanisms for $0 < \delta < 1/3$ and infinite-U points to the DMRG value[20] $\delta_{\mathrm{PS}}(U=\infty) \approx 0.225$ as the onset of the phase-separated regime: for $0 < \delta < \delta_{\mathrm{PS}}$ the Nagaoka mechanism dominates, whereas for $\delta_{\mathrm{PS}} < \delta < 1/3$ finite regions of the AB_2 chain present either fully polarized or singlet spin configurations. It is interesting to note that predictions for ladder[48] and square lattice[49] systems also estimate $\delta \approx 0.2$ as the upper hole density above which Nagaoka ferromagnetism becomes unstable.

C. Critical spin-1/2 antiferromagnetism at $\delta = 2/3$ and Luttinger-liquid behavior for $\delta > 2/3$

By hole doping the insulating short-range RVB states ($1/3 < \delta < 2/3$), DMRG results[20] have provided evidence of long-range pairing between single electrons located at well-separated unit cells (long-range RVB states). This crossover regime anticipates the emergence of Luttinger-liquid behavior for $\delta \geq 2/3$.[28] In particular, at commensurate doping $\delta = 2/3$ (one electron per unit cell) the system behaves similarly to a critical spin-1/2 antiferromagnetic linear chain at half filling,[10,29] with gapless spin excitations (in contrast to the spin-gapped case at $\delta = 1/3$) and charge gap satisfying a Lieb-Wu-type solution[30] that saturates to a finite value for $U = \infty$.[20] Actually, we first notice that for this hole doping in the infinite-U limit the degenerate states in the flat e band are not populated, so that the occupied energy spectra of $\delta = 2/3$ AB_2 and half-filled linear Hubbard chains are alike (recall that flat bands do not occur in linear Hubbard chains[10]). In addition, at $\delta = 2/3$ the single electron per AB_2 unit cell is equally distributed between A and $B_1 + B_2$ sites, i.e., $\langle n_A\rangle \approx \langle n_{B_1}\rangle + \langle n_{B_2}\rangle \approx 0.5$ on average (sum equals 1 in the unit cell), with antiferromagnetic correlation to the nearest spin.[20] By inserting these values of mean occupancy numbers into Eq. (54), and requiring the symmetry between B_1 and B_2 sites, we obtain

$$\mathcal{L}_{II} = \frac{1}{2}\sum_i \frac{i}{2}[-\mathbf{A}(\mathbf{n}_i) \cdot \partial_\tau \mathbf{n}_i + \mathbf{A}(\mathbf{n}_{i+1/2}) \cdot \partial_\tau \mathbf{n}_{i+1/2}]. \tag{55}$$

Therefore, as in the half-filled limit, the Wess-Zumino action becomes proportional to the topological winding number, Eq. (50). (However, in contrast to the $\delta = 0$ ferrimagnetic state, the ferromagneticlike Wess-Zumino counterpart vanishes for $\delta = 2/3$, as it happens for $\delta = 1/3$.) Apart from the 1/2 prefactor, Eq. (55) is identical to the Wess-Zumino term of strongly coupled linear Hubbard chains at half filling.[10,29] Similarly, infinite-U AB_2 Hubbard chains at hole doping $\delta = 2/3$ become critical, with power-law decay with distance of the spin-spin correlation function. *Stricto sensu*, as $J = 0$ in the infinite-U limit, it has been argued[50] that an infinitesimal

perturbation of order t/U must be present in order to remove the degeneracy of spin configurations at $U=\infty$, and give rise to the antiferromagnetically correlated ground state.

We now turn to the infinite-U regime with $\delta>2/3$ (less than one electron per cell on average). As the flat e band is empty, the effective Lagrangian (38) becomes

$$\begin{aligned}\mathcal{L}_\alpha = & \sum_i \alpha_i^\dagger \partial_\tau \alpha_i + \sum_i \alpha_i^{(1/2)\dagger} \partial_\tau \alpha_i^{(1/2)} \\ & + \sum_{i\sigma} \Bigg\{ \theta(-\sigma)(U_i^{(b)\dagger} \partial_\tau U_i^{(b)})_{\sigma\sigma} \alpha_i^{(1/2)\dagger} \alpha_i^{(1/2)} \\ & + \theta(\sigma) \frac{1}{2} \sum_{\nu=d,e} (U_i^{(\nu)\dagger} \partial_\tau U_i^{(\nu)})_{\sigma\sigma} \alpha_i^\dagger \alpha_i \Bigg\} \\ & - t \sum_{i\sigma} \{ \theta(-\sigma)(U_i^{(b)\dagger} U_i^{(d)})_{\sigma,-\sigma} \alpha_i^{(1/2)\dagger} \alpha_i \\ & + \theta(\sigma)(U_i^{(d)\dagger} U_{i+1}^{(b)})_{\sigma,-\sigma} \alpha_i^\dagger \alpha_{i+1}^{(1/2)} + \text{H.c.}\}. \end{aligned} \tag{56}$$

Notice that, since $\alpha_i^{(1/2)} \approx a_{iA\downarrow}$ and $\alpha_i \approx (a_{iB_1\uparrow} + a_{iB_2\uparrow})/\sqrt{2}$ in first order, and considering the definitions in Eq. (35), it is found that sites A and B_1+B_2 enter symmetrically in Lagrangian (56). Indeed, in the infinite-U limit exact-diagonalization results[20] have pointed to mean occupation numbers $\langle n_A \rangle \approx \langle n_{B_1} \rangle + \langle n_{B_2} \rangle$ also for $\delta>2/3$. Accordingly, the spin-spin correlation functions $\mathbf{S}_{iA}\cdot\mathbf{S}_{iB}$, $\mathbf{S}_{iA}\cdot\mathbf{S}_{i+1,A}$, and $\mathbf{S}_{iB}\cdot\mathbf{S}_{i+1,B}$, with $\mathbf{S}_{iB}=\mathbf{S}_{iB_1}+\mathbf{S}_{iB_2}$, display nearly the same magnitude, in contrast to their distinct values observed for $\delta<2/3$.[20] (The fact that $\mathbf{S}_{iB_1}\cdot\mathbf{S}_{iB_2}\approx 0$ is also consistent with the highly diluted regime for $\delta>2/3$; in contrast, it has been found that $\mathbf{S}_{iB_1}\cdot\mathbf{S}_{iB_2}<0$ in the presence of RVB singlet states for $1/3\leq\delta<2/3$.[20])

The absence of occupation of the flat band allows $\mathcal{L}_\alpha$ in Eq. (56) to be treated in a "squeezed chain" procedure.[12] We initially introduce spinless hole fields as $h_i^\dagger=\alpha_i$ and $h_i^{(1/2)\dagger}=\alpha_i^{(1/2)}$. Since $\alpha_i^\dagger\alpha_i=1-h_i^\dagger h_i$ and $\alpha_i^{(1/2)\dagger}\alpha_i^{(1/2)}=1-h_i^{(1/2)\dagger}h_i^{(1/2)}$, one readily sees that the contribution from hole sites to the Wess-Zumino term of Eq. (56) is null. Thus, with the help of Eq. (35), this term can be written as

$$\begin{aligned}\mathcal{L}_{\alpha,WZ} = & \sum_{i\sigma}{}' \Bigg\{ \theta(-\sigma)(U_{iA}^\dagger \partial_\tau U_{iA})_{\sigma\sigma} \\ & + \theta(\sigma)\frac{1}{2}[(U_{iB_1}^\dagger \partial_\tau U_{iB_1})_{\sigma\sigma} + (U_{iB_2}^\dagger \partial_\tau U_{iB_2})_{\sigma\sigma}] \Bigg\}, \end{aligned} \tag{57}$$

where Σ' indicates that the sum must be taken over occupied sites. Note that only spin degrees of freedom are present in Eq. (57). Moreover, the kinetic part of $\mathcal{L}_\alpha$ becomes

$$\begin{aligned}\mathcal{L}_{\alpha,kin} = & \sum_i h_i^\dagger \partial_\tau h_i + \sum_i h_i^{(1/2)\dagger} \partial_\tau h_i^{(1/2)} \\ & + t \sum_{i\sigma} \{ \theta(-\sigma)(U_i^{(b)\dagger} U_i^{(d)})_{\sigma,-\sigma} h_i^\dagger h_i^{(1/2)} \\ & + \theta(\sigma)(U_i^{(d)\dagger} U_{i+1}^{(b)})_{\sigma,-\sigma} h_{i+1}^{(1/2)\dagger} h_i + \text{H.c.}\}. \end{aligned} \tag{58}$$

Regarding the spin-rotation matrices $U_i^{(d)}$ and $U_i^{(b)}$, the absence of true spin (carried by the electron) at hole sites, along with their $U(1)$ local gauge freedom, allows to write[12] [see Eqs. (18)–(21)], without any loss of generality, $U_i^{(b)\dagger}U_i^{(d)} = U_i^{(d)\dagger}U_{i+1}^{(b)} = i\sqrt{2}\hat{\sigma}^x$ for such sites. Thus, as in the Nagaoka state, the hopping amplitudes assume their maximum values $\sqrt{2}$, and Eq. (58) reads

$$\begin{aligned}\mathcal{L}_{\alpha,kin} = & \sum_i h_i^\dagger \partial_\tau h_i + \sum_i h_i^{(1/2)\dagger} \partial_\tau h_i^{(1/2)} \\ & + t\sqrt{2} \sum_i [i h_i^\dagger h_i^{(1/2)} + i h_{i+1}^{(1/2)\dagger} h_i + \text{H.c.}]. \end{aligned} \tag{59}$$

In the squeezed chain procedure[12] an effective chain with a set of matrices $\{\tilde{U}_i^{(b)}, \tilde{U}_i^{(d)}\}$ can be obtained by removing all hole sites, where, according to the choice of B sites ahead of the A site within the unit cell,

$$U_i^{(b)} = \tilde{U}_i^{(b)} (i\hat{\sigma}^x)^{\Sigma_{\ell<i}[h_\ell^\dagger h_\ell + h_\ell^{(1/2)\dagger} h_\ell^{(1/2)}]},$$

$$U_i^{(d)} = \tilde{U}_i^{(d)} (i\hat{\sigma}^x)^{\Sigma_{\ell<i}[h_\ell^\dagger h_\ell + h_\ell^{(1/2)\dagger} h_\ell^{(1/2)}] + h_i^{(1/2)\dagger} h_i^{(1/2)}}. \tag{60}$$

In fact, the original chain with holes can be reproduced back from its squeezed counterpart by inserting the hole sites and the set $\{U_i^{(b)}, U_i^{(d)}\}$ as defined above. In addition, by considering $\tilde{h}_i = \exp(i\pi x_i) h_i$ and $\tilde{h}_i^{(1/2)} = \exp[i\pi(x_i - 1/2)] h_i^{(1/2)}$, one finally obtain the kinetic contribution to $\mathcal{L}_\alpha$ in the squeezed effective chain,

$$\begin{aligned}\mathcal{L}_{\alpha,kin} = & \sum_i \tilde{h}_i^\dagger \partial_\tau \tilde{h}_i + \sum_i \tilde{h}_i^{(1/2)\dagger} \partial_\tau \tilde{h}_i^{(1/2)} \\ & - t\sqrt{2} \sum_i [\tilde{h}_i^\dagger (\tilde{h}_{i+1}^{(1/2)} + \tilde{h}_i^{(1/2)}) + \text{H.c.}]. \end{aligned} \tag{61}$$

From Eqs. (57) and (61) we conclude that Lagrangian (56) can be expressed in a suitable representation where the spin and charge degrees of freedom are separated in the infinite-U limit, a feature also observed in doped linear Hubbard chains at $U=\infty$.[50] Indeed, as seen from Eq. (61), holes decouple from the spin background and move like free spinless fermions. The holon excitation spectrum is given by $\epsilon(k) = -2\sqrt{2}t\cos(k/2)$ and the ground-state energy coincides with that of Eq. (52).

It is interesting to compare these findings with the numerical evidence[20] of Luttinger-liquid behavior for $\delta\geq 2/3$ and infinite U, in which the spin-spin correlation function decays at long distances x as[7,12,50]

$$C(x) \sim \frac{\cos(2k_F x)[\ln(x)]^{1/2}}{x^{1+K_\rho}}; \tag{62}$$

above, k_F denotes the Fermi momentum and $K_\rho = \pi u_F/(2\chi)$, with Fermi velocity $u_F = \partial\epsilon/\partial k|_{k=k_F}$ and $\chi = V^{-1}\partial^2 E/\partial n_0^2$ ($n_0 = N_e/V$ is the electronic density and $V=N_c$ in the AB_2 case). By substituting the above results for E and ϵ, we obtain $K_\rho = 1/2$. We notice that this value is close to the ED results at $U=\infty$: $K_\rho=0.57$ for $\delta=88/106\approx 0.83$ and $K_\rho \to 1/2$ as $\delta \to 1$.[20] It is also worth mentioning that the exponent $K_\rho = 1/2$, originally derived at quarter filling, also holds for any electronic density below half filling (at which one finds $K_\rho = 0$).[7,50]

VII. DISCUSSION AND CONCLUSIONS

The present functional-integral formulation of the low-energy effective Lagrangian for the AB_2 Hubbard chains in the strong-coupling doped regime opens up the possibility to access analytically their rich phase diagram as a function of electron (or hole) density and Coulombian repulsion. Indeed, up to the present analytical works[15–17] have focused only on the half-filling point of the parameter space, whereas the remaining of it has been object of study through numerical techniques.[6,9,13,20–22]

In this sense, the approach to a number of relevant questions concerning the regime away from half filling now becomes feasible. Here we have focused on how the increasing doping in the AB_2 topology for infinite U manage to get from a ferromagnetic (Nagaoka) phase to a strongly coupled phase-separated regime, Mott-insulating RVB state at $\delta=1/3$, and Luttinger-liquid behavior for $\delta \geq 2/3$, with spin-charge separation.

Another issue of interest concerns the possibility of access to the quantum critical point of the quantum nonrelativistic nonlinear σ model,[17] related to half-filled strong-coupled AB_2 chains. Indeed, a RG analysis[17] indicates that the infrared behavior of quantum AB_2 ferrimagnetic Heisenberg chains with spin $S=1/2$ is driven by the $T=0$ semiclassical fixed point (coupling constant $g \propto 1/S=0$), with presence of long-range ground-state order (Lieb's theorem) and quantum (renormalized) corrections. The associated critical behavior as $T \to 0$ is similar to that[51] of the 1D quantum spin-1/2 Heisenberg ferromagnet and the organic ferromagnetic compound *p*-nitrophenyl nitroxyl nitroxide radical ($C_{13}H_{16}N_3O_4$), abbreviated as *p*-NPNN: susceptibility $\chi \sim T^{-2}$, correlation length $\xi \sim T^{-1}$, and specific heat $C \sim T^{1/2}$ driven by the spin-wave modes. These results have been confirmed[13] through exact diagonalization in the ferrimagnetic AB_2 Hubbard and Heisenberg chains. In contrast, the quantum critical low-T behavior at finite $g=g_c$ presents $\chi \sim T^{-1}$, $\xi \sim T^{-1/z}$, and $C \sim T^{d/z}$, with dynamical exponent $z=2$, similarly to the classical Heisenberg model in $d+z=3$ dimensions.[17] Since the coupling g relates to the magnitude of quantum fluctuations, any long-range ground-state order is destroyed for $g > g_c$. Interestingly, the same fixed-point structure has been found[52] in 1D itinerant electron systems in the context of a Luttinger-liquid framework. However, while in this case the localized spin-disordered phase is gapped, the quantum disordered phase in Ref. 52 behaves as an ordinary gapless Luttinger liquid. In this context, it has been argued[2] under which circumstances quantum AB_2 chains could approach such a strongly quantum disordered state and/or quantum critical behavior. Some suggestions consider the introduction of extra frustrated couplings in the unit-cell structure, although alternative scenarios involving other ingredients such as doping should not be discarded *a priori*.

In conclusion, we hope that the present formulation will allow further theoretical work to approach interesting questions regarding strongly coupled AB_2 Hubbard chains in the doped regime. The experimental counterpart, comprising inorganic and organic polymeric compounds, will certainly benefit from the improvement in the theoretical ground. In particular, we hope this work can stimulate more experimental research toward the exploration and understanding of the rich phase diagram of such quasi-1D compounds with AB_2 unit-cell structure, including the perspective of experimental discovery of rather interesting phases in the doped regime.

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