The ground state (GS) properties of the quasi-one-dimensional $AB_2$ Hubbard model are investigated taking the effects of charge and spin quantum fluctuations on equal footing. In the strong-coupling regime, we derive a low-energy Lagrangian suitable to describe the ferrimagnetic phase at half filling and the phases in the hole-doped regime. At half filling, a perturbative spin-wave analysis allows us to find the GS energy, sublattice magnetizations, and Lieb total spin per unit cell of the effective quantum Heisenberg model, in very good agreement with previous results. In the challenging hole doping regime away from half filling, we derive the corresponding $t$-$J$ Hamiltonian. Under the assumption that charge and spin quantum correlations are decoupled, the evolution of the second-order spin-wave modes in the doped regime unveils the occurrence of spatially modulated spin structures and the emergence of phase separation in the presence of resonating-valence-bond states. We also calculate the doping-dependent GS energy and total spin per unit cell, in which case it is shown that the spiral ferrimagnetic order collapses at a critical hole concentration. Notably, our analytical results in the doped regime are in very good agreement with density matrix renormalization group studies, where our assumption of spin-charge decoupling is numerically supported by the formation of charge-density waves in anti-phase with the modulation of the magnetic structure.

I. INTRODUCTION

Much attention has been given to quantum phase transitions [1, 2], which are phenomena characterized by the change of the nature of the ground state (GS) driven by a non-thermal parameter: pressure, magnetic field, doping, Coulomb repulsion, or competitive interactions. In this context, the study of quasi-one-dimensional (quasi-1D) compounds with ferrimagnetic properties [3, 4] has attracted considerable theoretical and experimental interest because of their unique physical properties and very rich phase diagrams. In particular, the GS of quasi-1D quantum ferrimagnets with $AB_2$ or $ABB'$ unit cell topologies (diamond or trimer chains) described by the Heisenberg or Hubbard models [5] exhibit unsaturated spontaneous magnetization, ferrimagnetic and antiferromagnetic spin-wave modes, effect of quantum fluctuations, and field-dependent magnetization plateaus, among several other features of interest.

Of special interest is the topological origin of GS magnetic long-range order associated with the unit cell structure of the lattice [5–12]. These studies have been motivated and supported by exact solutions and rigorous results [13–18]; in particular, at half filling, the total spin per unit cell obeys Lieb-Mattis [13] (Heisenberg model) or Lieb’s theorem [15] (Hubbard model). On the other hand, it has been verified that the ferrimagnetic GS of spin-1/2 Heisenberg and Hubbard/t-$J$ $AB_2$ chains, under the effect of frustration [19–23] or doping [7, 11, 24, 25], are strongly affected by quantum fluctuations that might cause its destruction and the occurrence of new exotic phases: spiral incommensurate (IC) spin structures, Nagaoka ($U \to \infty$) and resonating-valence-bond (RVB) states, phase separation (PS), and Luttinger-liquid behavior. These features can enhance the phenomenology in comparison with a linear chain, which is dominated by the nontrivial Luttinger-liquid behavior that exhibits fractional excitations [26, 27], emergent fractionalized particles [28], and fractional-exclusion statistic properties [29] in the spin-incoherent regime [30]. In addition, investigations of transport properties in $AB_2$ chains, and related structures, have also unveiled very interesting features [31].

On the experimental side, studies [32–34] of the magnetic properties of homometallic phosphate compounds of the family $A_2Cu_3(PO_4)_4$ ($A = Ca, Sr, Pb$) suggest that in these materials the line of trimers formed by spin-1/2 Cu$^{2+}$ ions antiferromagnetically coupled do exhibit ferrimagnetism of topological origin. Further, compounds $Ca_3M_3(PO_4)_4(M = Ni, Co)$ with a wave-like layer structure built by zigzag $M$-chains exhibit antiferromagnetic ordering ($M = Ni$) or paramagnetic behavior ($M = Co$) [35]. On the other hand, bimetallic compounds, such as $CuMn(S_2C_2O_2)_2 \cdot 7.5H_2O$ [36], can be modeled [36–38] by alternate spin-1/2 - spin-5/2 chains and support interesting field-induced quantum critical points and Luttinger-liquid phase [37]. In addition, frustrated diamond ($AB_2$ topology) chains can properly model the compound azurite, $Cu_3(CO_3)(OH)_2$, in which case the occurrence of the 1/3 magnetization plateau is verified at high fields [39] in agreement with topological arguments [40] akin to those invoked in the quantum Hall effect. The spin-1/2 trimer chain compound $Cu_3(P_2O_5OH)_2$, with antiferromagnetic interactions only, also display the 1/3 magnetization plateau [41]. Interestingly, it has been established that in azurite the magnetization plateau is a dimer-monomer state [42], i.e., the chain is formed by pairs of $S = 1/2$ monomers and $S = 0$ dimers, with a small local polarization of the diamond spins [43], in agreement with density functional theory [44]. These dimer-monomer states have been found previously in the context of modeling frustrated $AB_2$ chains [45–47], and confirmed through a modeling using quantum rotors [48]. In contrast to azurite, whose dimers appear perpendicular to the chain direction, in the spin-1/2 inequilateral diamond-chain compounds $A_2Cu_3Al_2O_3(SO_4)_4(A = K, Rb, Cs)$, the magnetic exchange interactions force the dimers to lie along the sides of the diamond cells and the monomers form a 1D
Heisenberg chain. In fact, the low-energy excitations of these new compounds have been probed and a Tomonaga-Luttinger spin liquid behavior identified [50]. It is worth mentioning that strongly frustrated $AB_2$ chains can exhibit ladder-chain decoupling [20], in which case the ladder is formed via the coupling between dimer spins in neighboring $AB_2$ unit cells.

On the other hand, besides the above-mentioned quasi-1D compounds and related magnetic properties, considerable efforts have been devoted to the study of superconductivity and intriguing magnetic/charge ordered phases in doped materials [51, 52], in particular the formation of spin-gapped states in compounds such as the family of doped (La, Sr, Ca)$_{14}$Cu$_{24}$O$_{11}$. This compound is formed by one-dimensional CuO$_2$ diamond chains, (Sr, Ca) layers, and two-leg Cu$_2$O$_3$ ladders [53]. These results certainly stimulate experimental and theoretical investigations of quasi-1D compounds in the hole-doped regime, which is the main focus of our work, as described in the following.

In this work, we shall employ an analytical approach suitable to describe the strongly coupled Hubbard model on doped $AB_2$ chains, which were the object of recent numerical studies through density matrix renormalization group (DMRG) techniques [25]. Our functional integral approach, combined with a perturbative expansion in the strong-coupling regime, was originally proposed to study the doped Hubbard chain [54], and later adapted to describe various doped-induced phase transitions in the $U = \infty AB_2$ Hubbard chain [55]. In addition, this approach was used to describe the doped strongly coupled Hubbard model on the honeycomb lattice [56], whose results are very rewarding, particularly those for the GS energy and magnetization in the doped regime, which compare very well with Grassmann tensor product numerical studies [57].

The paper is organized as follows: in Sec. II we review the functional integral representation of the Hubbard Hamiltonian in terms of Grassmann fields (charge degrees of freedom) and spin $SU(2)$ gauge fields (spin degrees of freedom). In Sec. III, we diagonalize the Hamiltonian associated with the charge degree of freedom and obtain a perturbative low-energy theory suitable to describe the ferrimagnetic phase at half filling and the phases in the hole-doped regimes. In Sec. IV, we show that the resultant Hamiltonian at half filling and large-$U$ maps onto the spin-1/2 quantum Heisenberg model. In this regime, a perturbative series expansions in powers of $1/S$ of the spin-wave modes is presented, which allows us to calculate the GS energy, sublattice magnetizations, and Lieb GS total spin per unit cell in very good agreement with previous estimates. In Sec. V, we derive the low-energy effective $t-J$ Hamiltonian, which accounts for both charge and spin quantum fluctuations. We also present the evolution of the second-order spin-wave modes, GS energy and total spin per unit cell under hole doping, thus identifying the occurrence of spatially modulated spin structures, with non-zero and zero GS total spin, and phase separation involving the later spin structure and RVB states at hole concentration 1/3. Remarkably, these predictions are in very good agreement with the DMRG data reported in Ref. [25]. Lastly, in Sec. VI, we present a summary and concluding remarks concerning the reported results.

### II. FUNCTIONAL-INTEGRAL REPRESENTATION

The Hamiltonian of the one-band Hubbard model on chains with $AB_2$ unit cell topology is given by [7, 8, 10]:

$$\mathcal{H} = -\sum_{\langle i, j \rangle \sigma} \{t^{\alpha \beta}_{ij} \hat{c}_{i \alpha \sigma} \hat{c}_{j \beta \sigma} + \text{H.c.} \} + U \sum_{\alpha} \hat{n}_{i \alpha \uparrow} \hat{n}_{i \alpha \downarrow},$$

where $i = 1, \ldots, N_c (= N/3)$ is the specific position of the unit cell, whose length is set to unity, $N_c (N)$ is the number of cells (sites), $\alpha, \beta = A, B_1, B_2$ denote the type of site within 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 $i$ of $\alpha$, and $\hat{n}_{i \alpha \sigma} = \hat{c}_{i \alpha \sigma} \dagger \hat{c}_{i \alpha \sigma}$ is the occupancy number operator. The first term in Eq. (1) describes electron hopping, with energy $t^{\alpha \beta} \equiv t$, allowed only between nearest neighbors $A-B_1$ and $A-B_2$ linked sites of sublattices $A$ and $B$ (bipartite lattice), and the second one is the on-site Coulombic repulsive interaction $U > 0$, which contributes only in the case of double occupancy of the site $i \alpha$.

At this point, it is instructive to digress on some fundamental aspects of the formalism used in our work [54–56]. With regard to the large-$U$ doped Hubbard chain [54], $U = \infty AB_2$ Hubbard chain [55] and the Hubbard model on the honeycomb lattice [56], it has been shown that the particle density product in Eq. (1) can be treated through the use of a decomposition procedure, which consists in expressing $\hat{n}_{i \alpha \uparrow} \hat{n}_{i \alpha \downarrow}$ in terms of charge and spin operators:

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

where

$$\hat{S}_{i \alpha} = 1/2 \sum_{\sigma \sigma'} c_{i \alpha \sigma} \sigma_{\alpha \sigma'} \sigma'_{i \alpha \sigma},$$

and

$$\hat{\rho}_{i \alpha} = \hat{n}_{i \alpha \uparrow} + \hat{n}_{i \alpha \downarrow},$$

are the spin-1/2 and charge-density operators, respectively, $\sigma_{\alpha \sigma}$ denotes the Pauli matrix elements ($h \equiv 1$), and $\hat{n}_{i \alpha}$ is an arbitrary unit vector. In fact, Eq. (2) follows from the identity:

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

The convenience of using the decomposition defined in Eq. (2), with explicit spin-rotational invariance for the large-$U$ Hubbard model, was discussed at length in Refs. [54–56].

We start by using the Trotter-Suzuki formula [58, 59], which allows us to write the partition function,

$$Z = \text{Tr} \{ \exp(-\beta \mathcal{H}) \},$$

at a temperature $k_B T \equiv 1/\beta$, as

$$Z = \text{Tr} \{ \hat{T} \prod_{r=1}^{M} \exp[-\delta r \mathcal{H}(\tau_r)] \},$$

where $\hat{T}$ denotes the time-ordering operator, the total imaginary time interval is formally sliced into $M$ discrete intervals of equal size $\delta r = \tau_r - \tau_{r-1}$, $r = 1, 2, ..., M$, with $\tau_0 = 0$, and $\tau_M = B \delta r$, under the limits $M \rightarrow \infty$ and $\delta r \rightarrow 0$. We shall now introduce, between each discrete time interval, an overcomplete basis of fermionic coherent states [58, 59],

$$\int \prod_{\alpha \sigma} dc_{i \alpha \sigma} \ exp \left\{ -\sum_{\alpha \sigma} c_{i \alpha \sigma} \dagger c_{i \alpha \sigma} \right\} \left\{ \{c_{i \alpha \sigma}\} \right\},$$

where $\{c_{i \alpha \sigma}\}$ is an overcomplete basis of coherent fermionic states.
where \( \{ c_{i\alpha\sigma}^\dagger, c_{i\alpha\sigma} \} \) denotes a set of Grassmann fields satisfying anti-periodic boundary conditions: \( c_{i\alpha\sigma}^\dagger(0) = -c_{i\alpha\sigma}^\dagger(\beta) \) and \( c_{i\alpha\sigma}(0) = -c_{i\alpha\sigma}(\beta) \); while the set of unit vectors defines the vector field \( \{ n_{i\alpha} \} \), satisfying periodic ones: \( n_{i\alpha}(0) = n_{i\alpha}(\beta) \), under a weight functional (see below). Thereby, following standard procedure [58, 59], the partition function reads:
\[
Z = \int \prod_{i\alpha\sigma} Dc_{i\alpha\sigma}^\dagger Dc_{i\alpha\sigma} \prod_i \prod_{\alpha\sigma} \mathcal{D}^2 n_{i\alpha} W(\{ n_{i\alpha} \}) e^{-\int_0^\beta \mathcal{L}(\tau) d\tau},
\]
where the pertinent measures are defined by
\[
Dc_{i\alpha\sigma}^\dagger Dc_{i\alpha\sigma} \equiv \lim_{M \to \infty, \delta \tau \to 0} \prod_{r=1}^{M-1} \prod_i \mathcal{D}c_{i\alpha\sigma}(\tau_r) \mathcal{D}c_{i\alpha\sigma}(\tau_r),
\]
\[
\mathcal{D}^2 n_{i\alpha} \equiv \lim_{M \to \infty, \delta \tau \to 0} \prod_{r=1}^{M-1} \mathcal{D}^2 n_{i\alpha}(\tau_r),
\]
the weight functional, \( W(\{ n_{i\alpha} \}) \), satisfies a normalization condition at each discrete imaginary time \( \tau_r \):
\[
\int \prod_{i\alpha} \mathcal{D}^2 n_{i\alpha} W(\{ n_{i\alpha}(\tau_r) \}) = 1,
\]
and the Lagrangian density \( \mathcal{L}(\tau) \) is written in the form:
\[
\mathcal{L}(\tau) = \sum_{i\alpha\sigma} c_{i\alpha\sigma}^\dagger \partial_\tau c_{i\alpha\sigma} - \sum_{ij\alpha\beta} \left( t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + \text{H.c.} \right) + U \sum_{i\alpha} \left( \rho_{i\alpha} - 2(n_{i\alpha} \cdot n_{i\alpha})^2 \right).
\]
In order to fix \( W(\{ n_{i\alpha} \}) \) one should notice, that in the operator formalism: \( \rho_{i\alpha}^2 = \hat{\rho}_{i\alpha} + 2n_{i\alpha}^2 \hat{n}_{i\alpha} \). Therefore, using Eq. (2), the following identity holds [54]:
\[
2(\hat{\mathbf{S}}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2 = \hat{\rho}_{i\alpha}(2 - \hat{\rho}_{i\alpha}) / 2,
\]
which means that the square of the spin component operator along the \( \mathbf{n}_{i\alpha} \) direction has zero eigenvalues if the site is vacant or doubly occupied, and a nonzero value only for singly occupied sites, i.e., \( (\hat{\mathbf{S}}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2 = 1/4 \). Now, taking advantage of the choice of \( n_{i\alpha} \), the local spin-polarization and spin-quantization axes are both chosen along the \( \mathbf{n}_{i\alpha} \) direction. Therefore, for singly occupied sites, we find \( \mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} = \rho_{i\alpha}/2 \), with \( \rho_{i\alpha} = \pm 1 \) corresponding to the two possible spin-1/2 states. Further, by incorporating vacancy and double occupancy possibilities, corresponding to the four possible local states of the Hubbard model, one can write [54]
\[
\rho_{i\alpha} \hat{\mathbf{S}}_{i\alpha} \cdot \mathbf{n}_{i\alpha} = \hat{\rho}_{i\alpha}(2 - \hat{\rho}_{i\alpha}) / 2,
\]
with \( \hat{\rho}_{i\alpha}^2 = (\pm 1)^2 \). We stress that, due to fermion operator properties, the square of Eq. (11) reproduces Eq. (10), and a comparison between them implies, at arbitrary doping and U value, the formal equivalence between \( 2(\hat{\mathbf{S}}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2 \) and \( \rho_{i\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} \). In this context, we remark that the original Coulomb repulsion term of the Hubbard Hamiltonian in Eq. (1) is formally and energetically (eigenvalues) equivalent to both that in Eq. (9) or in its linear version through the following replacement: \( 2(\hat{\mathbf{S}}_{i\alpha} \cdot \mathbf{n}_{i\alpha})^2 \to \rho_{i\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} \). Indeed, using the constraint in Eq. (11) we find, \( U \sum_{i\alpha} \left( \frac{\hat{\rho}_{i\alpha}}{\rho_{i\alpha}} - \rho_{i\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} \right) \), which is zero for \( \rho_{i\alpha} = 0, 1 \); whereas, as expected, for double occupied sites, \( \rho_{i\alpha} = 2 \), the local energy is \( U \). Therefore, Eq. (11) in its Grassmann version, can be enforced by a proper choice of the normalized weight functional:
\[
W(\{ n_{i\alpha} \}) = \lim_{M \to \infty, \delta \tau \to 0} \prod_{r=1}^M W(\{ n_{i\alpha}(\tau_r) \})
\]
\[
= C \exp \left\{- \int_0^\beta d\tau \sum_{i\alpha} \left[ \rho_{i\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} - \rho_{i\alpha}^2 (2 - \rho_{i\alpha})^2 \right] \right\},
\]
where \( \gamma \to \infty \) in the continuum limit \( (M \to \infty, \delta \tau \to 0) \), with delta-function peaks at the four local states of the Hubbard model, and \( C \) is a normalization factor such that Eq. (8) holds. In fact, the product of \( W(\{ n_{i\alpha}(\tau_r) \}) \) in Eq. (12) generates a sum in \( r \) in the exponential of the suitable chosen Gaussian function, i.e., \( W(\{ n_{i\alpha} \}) \) is such that in the continuum limit, \( M \to \infty, \delta \tau \to 0 \), Eq. (12) obtains with a diverging \( \gamma \), as pointed out in Ref. [54]. In this way, using Eq. (12) for the weight functional in Eq. (5) for the partition function \( Z \), and integrating over \( \{ n_{i\alpha} \} \), the Lagrangian density \( \mathcal{L}(\tau) \) in Eq. (9) can thus be written in the following linearized form [54]:
\[
\mathcal{L}(\tau) = \sum_{i\alpha\sigma} c_{i\alpha\sigma}^\dagger \partial_\tau c_{i\alpha\sigma} - \sum_{ij\alpha\beta} \left( t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + \text{H.c.} \right) + U \sum_{i\alpha} \left[ \rho_{i\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{n}_{i\alpha} \right],
\]
where the constraint in Eq. (11) was explicitly used.

Now, since we are interested in studying the GS properties of the \( AB_2 \) Hubbard chains, we choose the staggered factor \( \rho_{i\alpha} = 1 \) at sites \( \alpha \in \{ B_1, B_2 \} \), consistent with the long-range ferrimagnetic GS predicted by Lieb’s theorem at half filling and for any U value [7, 8, 15], in which case we assume broken rotational symmetry along the z-axis. In this context, by considering the symmetry exhibited by the ferrimagnetic order, let us define the SU(2)/U(1) unitary rotation matrix [60]
\[
U_{i\alpha} = \left[ \begin{array}{cc}
\cos \left( \frac{\theta_{i\alpha}}{2} \right) & -\sin \left( \frac{\theta_{i\alpha}}{2} \right) e^{-i\phi_{i\alpha}} \\
\sin \left( \frac{\theta_{i\alpha}}{2} \right) e^{i\phi_{i\alpha}} & \cos \left( \frac{\theta_{i\alpha}}{2} \right)
\end{array} \right],
\]
where \( \theta_{i\alpha} \) is the polar angle between the z-axis and the unit local vector \( \mathbf{n}_{i\alpha} \) and \( \phi_{i\alpha} \in [0, 2\pi) \) is an arbitrary azimuth angle due to the U(1) gauge freedom of choice for \( U_{i\alpha} \). Moreover, a new set of Grassmann fields, \( \{ a_{i\alpha\sigma}, a_{i\alpha\sigma}^\dagger \} \) can be obtained, according to the transformation:
\[
a_{i\alpha\sigma} = \sum_{\sigma'} (U_{i\alpha})_{\sigma\sigma'} a_{i\alpha\sigma'},
\]
that locally rotates each unit vector \( n_{i\alpha} \) to the \( z \)-direction. On the other hand, if we express the product \( \sigma \cdot n_{i\alpha} \) in matrix form:

\[
\sigma \cdot n_{i\alpha} = \begin{bmatrix}
\cos (\theta_{i\alpha}) & \sin (\theta_{i\alpha}) e^{-i\phi_{i\alpha}} \\
-\sin (\theta_{i\alpha}) e^{i\phi_{i\alpha}} & \cos (\theta_{i\alpha})
\end{bmatrix},
\]

(16)

we obtain, after using Eq. (14),

\[
U^\dagger_{i\alpha} (\sigma \cdot n_{i\alpha}) U_{i\alpha} = \sigma^z,
\]

(17)

which explicitly manifest the broken rotational symmetry along the \( z \)-axis. In this way, by substituting Eqs. (14) and (15) into Eq. (3), and using the above result, we find

\[
S_{i\alpha} \cdot n_{i\alpha} = \frac{1}{2} \sum_{\sigma\sigma'} a^\dagger_{i\alpha\sigma} U_{i\alpha} (\sigma \cdot n_{i\alpha}) U_{i\alpha\sigma'} a_{i\alpha\sigma'},
\]

\[
= \frac{1}{2} \sum_{\sigma\sigma'} a^\dagger_{i\alpha\sigma} (\sigma_z)_{\sigma\sigma'} a_{i\alpha\sigma'} \equiv S_{i\alpha}^z;
\]

(18)

thereby, the constraint in Eq. (11) can be written in the form

\[
S_{i\alpha} \cdot n_{i\alpha} = \rho_{i\alpha} (2 - \rho_{i\alpha}) = \frac{1}{2} (a^\dagger_{i\alpha\uparrow} a_{i\alpha\uparrow} - a^\dagger_{i\alpha\downarrow} a_{i\alpha\downarrow}),
\]

(19)

where \( \rho_{i\alpha} = +1 \) (-1) at sites \( \alpha = B_1, B_2 \) (\( A \)). The choice of \( \rho_{i\alpha} \) above implies Lieb’s ferrimagnetic ordering with the set \( \{ \theta_{i\alpha} = \theta_{i\beta} = \theta_{iB_2} = 0 \} \), for all \( \alpha \), at half filling. However, in the hole doped regime away from half filling, the \( \theta_{i\alpha} \)'s can be nonzero (e.g., \( \theta_{i\alpha} = \pi \) for a spin flip, leading to a change in the sign of \( S_{i\alpha}^z \)); further, \( S_{i\alpha}^z \) can be zero either by the presence of holes or doubly occupied sites \( a^\dagger_{i\alpha\uparrow} a_{i\alpha\uparrow} = a^\dagger_{i\alpha\downarrow} a_{i\alpha\downarrow} \).

Lastly, using Eqs. (15) and (19) into the Lagrangian, Eq. (13), we find, after suitable rearrangement of terms,

\[
\mathcal{L}(\tau) = \mathcal{L}_0(\tau) + \mathcal{L}_n(\tau),
\]

(20)

where both Lagrangians are quadratic in the Grassmann fields:

\[
\mathcal{L}_0(\tau) = \sum_{i\alpha\sigma} a^\dagger_{i\alpha\sigma} \partial_\tau a_{i\alpha\sigma} - \sum_{i\alpha\sigma,j\beta\sigma} (t^\beta_{ij} a^\dagger_{i\alpha\sigma} a_{j\beta\sigma} + \text{H.c.}) + U \sum_{i\alpha} \left(1 - p_{i\alpha}\sigma\right) a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma},
\]

(21)

and

\[
\mathcal{L}_n(\tau) = \sum_{i\alpha\sigma\sigma'} a^\dagger_{i\alpha\sigma} U_{i\alpha\sigma} \partial_\tau U_{i\alpha\sigma'} a_{i\alpha\sigma'}
\]

\[
- \sum_{i\alpha\sigma,j\beta\sigma'} t^\beta_{ij} a^\dagger_{i\alpha\sigma} U_{i\alpha\sigma} U_{j\beta\sigma'} - 1) a_{j\beta\sigma'} + \text{H.c.},
\]

(22)

with the first term in both Eqs. (21) and (22) being originated from the first term in Eq. (13), the second ones come from the hopping term in Eq. (13), after a rearrangement of terms, while the last one in Eq. (21) (proportional to \( U \)) is obtained by using Eq. (19) in the last term of Eq. (13). It is worth mentioning that only charge degrees of freedom (Grassmann fields) appear in \( \mathcal{L}_0(\tau) \), and spin degrees of freedom under the constraint in Eq. (19) \([SU(2)]\) gauge fields \( \{ U_{i\alpha}, U_{i\alpha} \} \), which carry all the information on the vector field \( \{ n_{i\alpha} \} \) are now restricted to \( \mathcal{L}_n(\tau) \), which includes both spin and charge degrees of freedom.

In the large-U regime, double occupancy is energetically unfavorable and the factor \( 2 - \rho_{i\alpha} \) is no longer needed in Eq. (19), i.e., \( S_{i\alpha} \cdot n_{i\alpha} = \rho_{i\alpha} \frac{\rho_{i\alpha}}{2} \), with \( \rho_{i\alpha} = 0 \) or 1. In this case, a proper perturbative analysis will allow us to study hole doping effects in Sec. \( V \) in a macroscopic fashion, so we define

\[
\delta = 1 - \frac{1}{N} \sum_{i\alpha} \langle \rho_{i\alpha} \rangle,
\]

(23)

which measures the thermodynamic average of hole doping away from half filling. In this context (strong-coupling limit), we take advantage of results derived from \( \mathcal{L}_0(\tau) \) (charge effects in Sec. \( III \)), and at half filling (Sec. \( IV \)), in which case charge degrees of freedom are frozen.

III. CHARGE DEGREES OF FREEDOM AND THE STRONG-COUPLING LIMIT

In this section, we shall first diagonalize the Hamiltonian associated with the Lagrangian \( \mathcal{L}_0(\tau) \) through the use of a special symmetry property of the \( AB_2 \) chains and a canonical transformation in reciprocal space. Then, by introducing a perturbative expansion in the strong-coupling regime, a low-energy effective Lagrangian for the \( AB_2 \) Hubbard chains at half filling and in the doped regime will be obtained.

A. Charge degrees of freedom

We begin our discussion by considering the Lagrangian \( \mathcal{L}_0 \) in Eq. (21), and its corresponding Hamiltonian \( \mathcal{H}_0 \), free of the \( SU(2) \) gauge fields. By performing the Legendre transformation: \( \mathcal{H}_0 = - \sum_{i\alpha\sigma} \partial_{\partial_\tau a_{i\alpha\sigma} a_{i\alpha\sigma}} \mathcal{L}_0 + \mathcal{L}_0 \), where \( \partial_{\partial_\tau a_{i\alpha\sigma}} \mathcal{L}_0 = a^\dagger_{i\alpha\sigma} \), the resulting \( \mathcal{H}_0 \) is given by

\[
\mathcal{H}_0 = - \sum_{i\alpha,j\beta} \langle t^\beta_{ij} a^\dagger_{i\alpha\sigma} a_{j\beta\sigma} + \text{H.c.} \rangle
\]

\[
+ U \sum_{i\alpha} \left(1 - p_{i\alpha}\sigma\right) a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma}.
\]

(24)

Further, since \( \mathcal{H}_0(\mathcal{L}_0) \) is quadratic in the Grassmann fields, the solution for the energy of the system is given by \( \mathcal{H}_0 \) in its diagonalized form \([59]\).

The \( AB_2 \) unit cell topology exhibits a symmetry \([9, 11, 24, 25, 55]\) under the exchange of the labels of the \( B \) sites in a given unit cell. Thus, we can construct a new set of Grassmann fields possessing this symmetry, i.e., either symmetric or antisymmetric with respect to the exchange operation \( B_1 \leftrightarrow B_2 \):

\[
(d_{i\sigma}, e_{i\sigma}) = \frac{1}{\sqrt{2}} (a_{iB_1\sigma} \pm a_{iB_2\sigma}), \quad b_{i\sigma} = a_{iA\sigma}.
\]

(25)
In addition, as a signature of the quasi-1D structure of the $AB_2$ chains, we notice that the $B_1$ and $B_2$ sites are located at a distance $1/2$ (in units of length) ahead of the $A$ site. Therefore, after Fourier transforming the above Grassfeld systems, i.e., $\{d_{i,\sigma}, e_{i,\sigma}, b_{i,\sigma}\} = \frac{1}{\sqrt{N_c}} \sum_k e^{ikx_i} \{d_{k,\sigma}, e_{k,\sigma}, b_{k,\sigma}\}$, it is convenient to introduce a phase factor $e^{ixk}$ through the following transformation [55]: $(A_{k,\sigma}, B_{k,\sigma}) = \frac{1}{\sqrt{2}} (d_{k,\sigma} \pm e^{ixk} b_{k,\sigma})$, so that $\mathcal{H}_0$ in Eq. (24) thus becomes

\[
\mathcal{H}_0 = \sum_{k,\sigma} \varepsilon_k [A_{k,\sigma}^\dagger A_{k,\sigma} - B_{k,\sigma}^\dagger B_{k,\sigma}] + \frac{U}{2} \sum_{k,\sigma} (1 - \sigma) e_k^\dagger e_k^\sigma,
\]

with $k = 2\pi j(N/2) - \pi$, and $j = 1, \ldots, N/3$. We can now exactly diagonalize $\mathcal{H}_0$ through the following Bogoliubov transformation:

\[
A_{k,\sigma} = u_k a_{k,\sigma} - \sigma v_k b_{k,\sigma}, \quad B_{k,\sigma} = \sigma v_k a_{k,\sigma} + u_k b_{k,\sigma},
\]

with $u_k$ and $v_k$ satisfying the canonical constraint: $(u_k)^2 + (v_k)^2 = 1$, to maintain the anticommutation relations of the Grassfeld fields. Due to the fermionic order of the GS, the above transformation is subject to a $4\pi$ periodicity of the Bogoliubov functions $\{u_k, v_k\}$ and Grassfeld fields $\{a_{k,\sigma}, b_{k,\sigma}\}$. The diagonalized $\mathcal{H}_0$ thus reads:

\[
\mathcal{H}_0 = - \sum_{k,\sigma} (E_k - \frac{U}{2}) a_{k,\sigma}^\dagger a_{k,\sigma} + \sum_{k,\sigma} (E_k + \frac{U}{2}) b_{k,\sigma}^\dagger b_{k,\sigma}
+ \frac{U}{2} \sum_{k,\sigma} (1 - \sigma) e_k^\dagger e_k^\sigma,
\]

where

\[
(u_k, v_k) = \frac{1}{\sqrt{2}} \left(1 \pm \frac{\varepsilon_k}{E_k}\right)^{1/2},
\]

and

\[
E_k = \sqrt{\varepsilon_k^2 + U^2}/4.
\]

As one can see from Eq. (29), the non-interacting tight binding ($U = 0$) spectrum of $\mathcal{H}_0$ present three electronic bands: a nondispersive flat band (related to the Grassfeld fields $\{e_{k,\sigma}, e_{k\sigma}\}$), macroscopically degenerate, and two dispersive ones. In $AB_2$ chains, flat bands are closely associated with ferrimagnetism (unsaturated ferromagnetism) [5, 7, 8] at half filling, in agreement with Lieb’s theorem [15, 16], or fully polarized ferromagnetism [17] associated with the flat lowest band. We also stress that even at this level of approximation and in the weak coupling regime ($U = 2t$), it was shown [7] that hole doping [parametrized by $\delta$ defined in Eq. (23)] can destroy the ferrimagnetic order and/or induce phase separation in $AB_2$ chains. As depicted in Fig. 1(a), the $U = 0$ spin degeneracy of the flat bands is removed by the Coulombian repulsive interaction, in which case a gap $U$ opens between the $e_{k,\sigma}$ modes: $e_{k,\uparrow} = 0$, where spins at sites $B_1$ and $B_2$ are up, and $e_{k,\downarrow} = U$, where these spins are down. On the other hand, the two dispersive bands are spin degenerated, and also display a Hubbard gap $U$ separating the low ($\alpha_{k,\sigma}$)-energy and high ($\beta_{k,\sigma}$)-energy modes [55].

### B. Strong-coupling limit

In this subsection, we shall introduce a perturbative expansion in the strong-coupling regime ($U \gg t$) in order to obtain a low-energy effective Lagrangian for the $AB_2$ Hubbard chain at half filling and in the doped regime. First, we resume the results of the previous section by writing the Grassfeld fields $d_{i,\sigma}$ and $b_{i,\sigma}$ in terms of the Grassfeld (Bogoliubov) fields $a_{i,\sigma}$ and $b_{i,\sigma}$:

\[
(d_{i,\sigma}, b_{i,\sigma}) = \frac{1}{\sqrt{2N_c}} \sum_k (e^{ikx_i}, e^{ik(x_i - t/2)}) \times [(u_k \pm \sigma v_k) a_{k,\sigma} \pm (u_k + \sigma v_k) b_{k,\sigma}],
\]

where the phase factor $e^{ik\sigma}$ signalizes the quasi-1D $AB_2$ structure, and the antisymmetric Grassfeld field $e_{i,\sigma}$ remains as defined in Eq. (25). In the strong-coupling limit, however, it will prove useful to define a set of auxiliary spinless Grassfeld fields $\{\alpha_{k,\sigma}, \beta_{k,\sigma}\}$:

\[
(\alpha_i, \beta_i) = \sqrt{\frac{TN_c}{2}} \sum_{k,\sigma} \theta(\pm \sigma) e^{ikx_i} (\alpha_{k,\sigma}, \beta_{k,\sigma}),
\]

and a similar equation for $(\alpha_i^\dagger, \beta_i^\dagger) \leftrightarrow (\alpha_{k,\sigma}, \beta_{k,\sigma})$ is obtained by the replacements: $\theta(\pm \sigma) \rightarrow \theta(\mp \sigma)$ and $x_i \rightarrow x_i - 1/2$, where $\theta(\sigma)$ is the Heaviside function, while for the antisymmetric component, one has

\[
e_{i,\sigma} = \sqrt{\frac{TN_c}{2}} \sum_k e^{ikx_i} e_{k,\sigma}.
\]

Now, by expanding $(u_k, v_k)$ in Eq. (30) in powers of $t/U$:

\[
(u_k, v_k) \approx \frac{1}{\sqrt{2}} \left(1 \pm \frac{\varepsilon_k}{E_k}\right) + \mathcal{O}\left(\frac{t^2}{U^2}\right),
\]

substituting these results into the Eq. (32), and using the inverse transformation of Eq. (33), we can derive a perturbative expansion in powers of $t/U$ for the Grassfeld fields $d_{i,\sigma}$ and $b_{i,\sigma}$ in terms of the spinless Grassfeld fields as follows:

\[
d_{i,\sigma} = \theta(\sigma) a_i + \theta(-\sigma) b_i + \sqrt{\frac{4t}{U}} \theta(\sigma) (\alpha_i^\dagger + \beta_i^\dagger)
+ \frac{t}{U} \theta(\sigma) \left[\beta_i^\dagger + \beta_{i+1}^\dagger - \frac{t}{U} (2\alpha_i + \alpha_{i+1} + \alpha_{i-1})\right]
+ \mathcal{O}(t^2/U^2),
\]

(36)
In the above derivation, we have used that $\theta(\sigma)\theta(\sigma^\prime) = \theta(\sigma)\delta_{\sigma,\sigma^\prime}$. Notice that, since $\frac{t}{U} \ll 1$, in Eqs. (36) and (37) we can identify the fields $\alpha_\theta^\frac{1}{2} \approx a_{iA\uparrow}$ and $\alpha_i \approx (a_{iB\uparrow} + a_{iB\downarrow})/\sqrt{2}$, a result fully consistent with the low-energy spin configuration of the ferrimagnetic state discussed previously. Analogously, for the high-energy bands, the opposite spin configuration is observed, with spin up (down) present at sites $A(B_1, B_2)$.

Introducing Eqs. (36) and (37) into Eq. (24), with the aid of Eq. (25), we obtain a perturbative expression for $\mathcal{H}_0$ (low-energy sector) in terms of the spinless Grassmann fields up to order $J = 4t^2/U$:

$$\mathcal{H}_0 = -J \sum_i [\alpha_i^\dagger \alpha_i + \alpha_i^{(\frac{1}{2})\dagger} \alpha_i^\frac{1}{2} - \beta_i^\dagger \beta_i - \beta_i^{(\frac{1}{2})\dagger} \beta_i^\frac{1}{2}]$$

$$- \frac{J}{2} \sum_i [\alpha_i^\dagger \alpha_{i+1} + \alpha_i^{(\frac{1}{2})\dagger} \alpha_{i+1}^\frac{1}{2} - \beta_i^\dagger \beta_{i+1} - \beta_i^{(\frac{1}{2})\dagger} \beta_{i+1}^\frac{1}{2}] + U \sum_i [\beta_i^\dagger \beta_i + \beta_i^{(\frac{1}{2})\dagger} \beta_i^\frac{1}{2} + e_i^\dagger e_i].$$

By applying Fourier transform to the above expression and rearranging the terms, we obtain

$$\mathcal{H}_0 = -\sum_k 2J \cos^2(k/2) (\alpha_k^\dagger \alpha_k + \alpha_k^{(\frac{1}{2})\dagger} \alpha_k^\frac{1}{2})$$
$$+ \sum_k [2J \cos^2(k/2) + U] (\beta_k^\dagger \beta_k + \beta_k^{(\frac{1}{2})\dagger} \beta_k^\frac{1}{2})$$
$$+ \frac{U}{2} \sum_{k\sigma} (1 - \sigma) e_k^\dagger e_{k\sigma}.$$  

In Fig. 1 we plot the electronic spectrum of the Hamiltonian $\mathcal{H}_0$, both in the weak and strong-coupling regime: (a) Eq. (29) for $U = 2t$ and (b) Eqs. (29) and (39) for $U = 12t$ ($J = 4t^2/U = 1/3$), respectively, with $t \equiv 1$. We can notice the presence of the shrinking phenomenon [7] as $U$ increases from $2t$ to $12t$ (strong-coupling regime) and that, for $U = 12t$, Eq. (39) is a very good approximation to Eq. (29). Noticeably, the $t \ll U$ expansion of the fields allows us to identify $\alpha_k^\frac{1}{2} \approx a_{kA\uparrow}$, $\alpha_k \approx (a_{kB\uparrow} + a_{kB\downarrow})/\sqrt{2}$ (triplet state) and $e_k^{\dagger} \approx (a_{kB\uparrow} - a_{kB\downarrow})/\sqrt{2}$ (singlet state), as the low-energy spin configuration of the ferrimagnetic state with single occupancy, where spins at sites $A(B_1, B_2)$ are down (up), in agreement with Lieb's theorem [15].

We shall now focus on the $U \gg t$ perturbative expansion of $\mathcal{L}_0$, Eq. (22), which amounts to consider the most significant low-energy processes, after the use of Eqs. (36) and (37) for $\alpha_{i\sigma}$ and $b_{i\sigma}$ in terms of the spinless Grassmann fields. However, terms allowing interband transitions between low- and high-energy bands do exist in $\mathcal{L}_0$. In this context, we apply a suitable second-order Rayleigh-Schrödinger perturbation theory [54, 55], consistent with the strong-coupling expansion, so that the modes associated with the high-energy bands are eliminated. Lastly, by adding $\mathcal{L}_0$ to the perturbative expansion of $\mathcal{L}_0$, which leads to the cancellation of the exchange terms in Eq. (40), the effective low-energy Lagrangian density of the $AB_2$ Hubbard model in the strong-coupling limit (up to order $J$) reads:

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

where

$$\mathcal{L}^{(I)} = \sum_i \alpha_i^\dagger \partial_\tau \alpha_i + \sum_i \alpha_i^{(\frac{1}{2})\dagger} \partial_\tau \alpha_i^{\frac{1}{2}} + \sum_i e_i^\dagger \partial_\tau e_i.$$
\( \mathcal{L}^{(I)} = \sum_{i,\sigma} \left\{ \theta(-\sigma)(U_i^{(b)})_{\sigma,\sigma} \partial_t U_i^{(b)} + (U_i^{(b)})_{\sigma,\sigma} \partial_t U_i^{(b)} \right\} \)

\[
\begin{align*}
L_{\text{eff}} &= \sum_{i,\sigma} \left\{ \theta(\sigma) \left[ (U_i^{(d)})_{\sigma,\sigma} \alpha_i^{(2)} \frac{1}{2} \alpha_i^{(2)} + \theta(\sigma) \left( \frac{1}{2} \partial_t U_i^{(d)} + \partial_t U_i^{(c)} \right)_{\sigma,\sigma} \right] \right. \\
&\quad \times (\alpha_i^{(2)} \alpha_i^{(2)} + e_i^{(2)} e_i^{(2)} + \theta(\sigma) \left( \frac{1}{2} \partial_t U_i^{(d)} + \partial_t U_i^{(c)} \right)_{\sigma,\sigma}) + \left. \left( U_i^{(c)} \partial_t U_i^{(d)} \right)_{\sigma,\sigma} | \alpha_i^{(2)} \alpha_i^{(2)} + \text{H.c.} \right\},
\end{align*}
\]

(42b)

\[
L^{(III)} = -J \sum_{i,\sigma} \theta(\sigma)(U_i^{(d)})_{\sigma,\sigma} \alpha_i^{(2)} \alpha_i^{(2)} + \theta(\sigma)(U_i^{(d)})_{\sigma,\sigma} \alpha_i^{(2)} \alpha_i^{(2)}
\]

(42c)

\[
L^{(IV)} = -J \sum_{i,\sigma} \theta(\sigma)(U_i^{(d)})_{\sigma,\sigma} \alpha_i^{(2)} \alpha_i^{(2)}
\]

(42d)

in which case we took advantage of the symmetry of the AB chain under the exchange operation \( B_1 \leftrightarrow B_2 \), in correspondence with Eq. (25). From the above equations, we see that the kinetic term is represented by \( L^{(I)} \) and is related to the charge degrees of freedom only, whereas \( L^{(III)} \) describes the dynamics of the spin degrees of freedom coupled to the charge fields. On the other hand, \( L^{(IV)} \) exhibit first-neighbor hopping contributions between charge degrees of freedom in the presence of \( SU(2) \) gauge fields, while \( L^{(IV)} \) is the spin exchange term in the presence of the charge Grassmann fields.

IV. HALF-FILLING REGIME

Let us now discuss some basic aspects of the localized magnetic properties related to the spin degrees of freedom. At half filling, i.e., \( \delta = 0 \), we have \( \langle \alpha_i^\dagger \alpha_i \rangle = 1 \), \( \langle \alpha_i^{(1/2)^\dagger} \alpha_i^{(1/2)} \rangle = 1 \), \( \langle e_i^\dagger e_i \rangle = 1 \), and \( \langle e_i^{(2)} e_i^{(2)} \rangle = 0 \) (no band hybridization) as the electrons tend to fill up the lower-energy bands, whereas the higher-energy ones remain empty. As a consequence, a ferromagnetic configuration of localized spins emerges, i.e., the charge degrees of freedom are completely frozen, such that \( \langle \alpha_i^\dagger \partial_t \alpha_i \rangle = \langle \alpha_i^{(1/2)^\dagger} \partial_t \alpha_i^{(1/2)} \rangle = \langle e_i^\dagger \delta_t e_i \rangle = 0 \), with forbidden hopping. Therefore, only terms from \( L^{(I)} \) and \( L^{(IV)} \) in Eqs. (42b) and (42d), respectively, give nonzero contributions and the resulting effective strong-coupling Lagrangian at half filling, defined in Eq. (41), reads:

\[
L_{\text{eff}}^J = \sum_{i,\sigma} \theta(p_{i\sigma})(U_i^{\dagger \sigma} \partial_t U_{i\sigma} + \text{H.c.}) - \frac{J}{4} \sum_{i,\sigma} \theta(p_{i\sigma}) \left| (U_i^{\dagger \sigma} \partial_{t \sigma} U_{i\sigma} + \text{H.c.}) \right|^2,
\]

(44)

where the staggered factor \( p_{i\sigma} \) was defined in Eq. (11), and use was made of the matrix transformations defined in Eq. (43) in order to sum up the squares of the \( SU(2) \) gauge field products in the exchange contribution from \( L^{(IV)} \) in Eq. (42d).

Now, using the following Legendre transform:

\[
\mathcal{H}_{\text{eff}}^J = -\sum_{i,\sigma} \frac{\partial L_{\text{eff}}^J}{\partial (U_i^{\dagger \sigma} \partial_t U_{i\sigma})} \frac{\partial L_{\text{eff}}^J}{\partial (U_i^{\dagger \sigma} \partial_t U_{i\sigma})} + \mathcal{H}_{\text{eff}}^J = \theta(p_{i\sigma})(U_i^{\dagger \sigma} \partial_{t \sigma} U_{i\sigma} + \text{H.c.}) \]

we get the respective quantum Heisenberg Hamiltonian written in terms of the \( SU(2) \) gauge fields at half filling as

\[
\mathcal{H}_{\text{eff}}^J = -\frac{J}{4} \sum_{i,\sigma} \theta(p_{i\sigma}) \left| (U_i^{\dagger \sigma} \partial_{t \sigma} U_{i\sigma}) \right|^2.
\]

(45)

Further, using the definition of the \( SU(2)/U(1) \) unitary rotation matrix Eq. (14), it is possible to write [54–56]

\[
\left| (U_i^{\dagger \sigma} \partial_{t \sigma} U_{i\sigma}) \right|^2 = \frac{1}{2}(1 + n_{i\sigma} \cdot n_{j\beta}),
\]

where \( n_{i\sigma} = \sin(\theta_{i\sigma}) \hat{x} + \sin(\phi_{i\sigma}) \hat{y} + \cos(\theta_{i\sigma}) \hat{z} \) is the unit vector pointing along the local spin direction. Lastly, by using the constraint as given in Eq. (19), we can identify the spin field \( \{ S_{i\sigma} \} \) at the single occupied sites:

\[
S_{i\sigma} = p_{i\sigma} n_{i\sigma}/2,
\]

(46)

where \( p_{i\sigma} = +1 (-1) \) at sites \( \sigma = B_1, B_2 (A) \), in order to obtain

\[
\mathcal{H}_{\text{eff}}^J = J \sum_i \left[ (S_i^{B_1} + S_i^{B_2}) \cdot (S_i^A + S_i^{A+1}) \right] - JN_c.
\]

(47)

The above expression is indeed that of the quantum antiferromagnetic Heisenberg spin-1/2 model on the \( AB \) chain in zero-field, which takes into account the effects of zero-point quantum spin fluctuations. In fact, to achieve this goal, we analyze the Hamiltonian, Eq. (47), by means of the spin-wave theory, which has proved very successful in describing the properties of the GS and low-lying excited states of spin models. The predicted results provide a check of the consistency of our approach and will be fully used in our description of the doped regime.

We shall first introduce boson creation and annihilation operators via the Holstein-Primakoff [58] transformation:

\[
S_i^{A+} = S_i^A + a_i^\dagger a_i,
\]

\[
S_i^{A-} = (S_i^{A+})^\dagger = \sqrt{2S} a_i^\dagger f_A(S),
\]

(48)

for a down-spin on the A site, and

\[
S_i^{B_1+} = S_i^{B_1} - b_i^\dagger b_i,
\]

\[
S_i^{B_1-} = (S_i^{B_1+})^\dagger = \sqrt{2S} f_B(S) b_i,
\]

(49)
for an up-spin on the $B_1$ site, with $l = 1, 2,$ and

$$f_r(S) = \left(1 - \frac{2n_r}{2S}\right)^{1/2} = 1 - \frac{1}{2S} + \ldots,$$  

where $S$ is the spin magnitude, and $n_r = a^\dagger_1 a_1$ or $b^\dagger_1 b_1$. The operators $a_1^\dagger$ and $a_1$ (or $b_1^\dagger$, $b_1$) satisfy the boson commutation rules. Under the above transformation, the spin Hamiltonian, Eq. (47) is mapped onto the boson Hamiltonian:

$$\mathcal{H}_{eff}^J = E_0 - J N_c + \mathcal{H}_1 + \mathcal{H}_2 + O(S^{-1}),$$  

where

$$E_0 = -4S^2 J N_c,$$  

is the classical GS energy and $\mathcal{H}_1$ and $\mathcal{H}_2$ are the quadratic and quartic (interacting) terms of the boson Hamiltonian, suitable to describe the quantum $AB_2$ Heisenberg model via a perturbative series expansion in powers of $1/S$. By Fourier transforming the boson operators, we find

$$\mathcal{H}_1 = 2JS \sum \langle 2a^\dagger_ka_k + \sum b^\dagger_kb_{lk} \rangle + \sum_{k,l=1,2} 2JS\gamma_k(a^\dagger_k b_{lk} + a_kb_{lk}),$$  

where we have defined the lattice structure factor as

$$\gamma_k = \frac{1}{z} \sum_{\rho} e^{ik\rho} = \cos \left(\frac{k}{2}\right),$$  

with $z$ denoting the coordination number ($z = 4$ for the $AB_2$ chain), while $\rho = \pm 1/2$ connects the nearest neighbors $A-B_1$ and $A-B_2$ linked sites of sublattices $A$ and $B$, and

$$\mathcal{H}_2 = -\frac{3J}{2N} \sum_{1234, l=1,2} \delta_{1234} \left\{ 4\gamma_{1-4} a^\dagger_1 a_4 b^\dagger_3 b_2 + (\gamma_{1+2-3} a^\dagger_1 a_3 a^\dagger_2 a_3 b^\dagger_{14} + \text{H.c.}) \right\}. $$  

For simplicity, we use the convention 1 for $k_1$, 2 for $k_2$, and so on. Also, the $\delta_{1234} = \delta(k_1 + k_2 - k_3 - k_4)$ is the Kronecker $\delta$ function, and expresses the conservation of momentum to within a reciprocal-lattice vector $G$.

We shall consider $\mathcal{H}_1$ first, which is the term leading to linear spin-wave theory (LSWT). In fact, $\mathcal{H}_1$ is diagonalized using the following Bogoliubov transformation:

$$a_k = u_k \beta_k - v_k \alpha^\dagger_k,$$

$$b_{lk} = \frac{1}{\sqrt{2}}[u_k \alpha_k - v_k \beta_k + (1)^j \xi_k],$$  

with $l = 1, 2,$

$$\langle u_k, v_k \rangle = \frac{(3 + \sqrt{9 - 8\gamma_k})}{\sqrt{3 + \sqrt{9 - 8\gamma_k}^2 - 8\gamma_k}},$$  

where $u_k$ and $v_k$ satisfy the constraint $u_k^2 - v_k^2 = 1$. Thus,

$$\mathcal{H}_1 = E_1 + \sum_k (\epsilon_k^0(\alpha) \alpha_k^\dagger \alpha_k + \epsilon_k^0(\beta) \beta_k^\dagger \beta_k + \epsilon_k^0(\xi) \xi_k^\dagger \xi_k);$$  

$$E_1 = JS \sum_k (\sqrt{9 - 8\gamma_k^2} - 3),$$

$$\epsilon_k^0(\alpha) = JS(\sqrt{9 - 8\gamma_k^2} + 1), \quad \epsilon_k^0(\xi) = 2JS,$$

where $E_1$ is the $O(S^1)$ quantum correction to the GS energy, and $\epsilon_k^0(\alpha), \epsilon_k^0(\xi)$ are the three spin-wave branches provided by LSWT, both in agreement with previous results [19, 61]. In fact, it is well known that systems with a ferrimagnetic GS naturally have ferromagnetic and antiferromagnetic spin-wave modes as their elementary magnetic excitations (magnons). For the $AB_2$ chain, there are three spin-wave branches: an antiferromagnetic mode $\epsilon_k^0(\beta)$, and two ferromagnetic ones $\epsilon_k^0(\alpha)$ and $\epsilon_k^0(\xi)$. The mode $\epsilon_k^0(\alpha)$ is gapless at $k = 0$, i.e., the Goldstone mode, with a quadratic (ferromagnetic) dispersion relation $\epsilon_k^0(\alpha) \sim k^2$. The other two modes are gapped. Notice that the gapped ferromagnetic mode $\epsilon_k^0(\xi)$ is flat, and is closely associated with ferromagnetic properties at half filling [7, 17]. Since the dispersive modes preserve the local triplet bond, they are identical to those found in the spin-1/2 - spin-1 chains [62–65]. These chains also exhibit interesting field-induced Luttinger liquid behavior [66].

Now, our aim is to obtain the leading corrections to LSWT, i.e., second-order spin-wave theory to the GS energy, sublattice magnetizations and Lieb GS total spin per unit cell. In doing so, we develop a perturbative scheme for the description of this quartic term. First, we decompose the two-body terms by means of the Wick theorem, via normal-ordering protocol for boson operators. Conservation of momentum to within a reciprocal-lattice vector, implies: $k_1 = k + q$, $k_2 = p - q$, $k_3 = k$ and $k_4 = p$. Then, we need to look at the possible pairings of the 4 operators, as for example, in the first term of Eq. (55):

$$a^\dagger_{k+q} a^\dagger_{l+p} b^\dagger_{l+p} b_{k-p}, \quad a^\dagger_{k+q} a^\dagger_{k+q} b^\dagger_{k+p} b_{l+p}, \quad a^\dagger_{k+q} a^\dagger_{k+q} b^\dagger_{l-p} b_{l+p}.$$

Under this procedure, and by substituting the Bogoliubov transformation, Eqs. (56)-(57), into Eq. (55), we find

$$\mathcal{H}_2 = E_2 + \sum_k (\delta\epsilon_k^\alpha \alpha_k^\dagger \alpha_k + \delta\epsilon_k^\beta \beta_k^\dagger \beta_k + \delta\epsilon_k^\xi \xi_k^\dagger \xi_k),$$  

where

$$E_2/N_c = -2J(q_1^2 + q_2^2 - \frac{3}{\sqrt{2}} q_1 q_2),$$  

and the corresponding corrections for the spin-wave dispersion relations read:

$$\delta\epsilon_k^\alpha = J[u_k^2(\sqrt{2}q_2 - 2q_1) + 2v_k^2(\sqrt{2}q_2 - q_1)] + 4J\gamma_k u_k v_k \left(\frac{3}{2\sqrt{2}} q_1 - q_2\right) + O(S^{-1}),$$  

$$\delta\epsilon_k^\beta$$ is obtained from $\delta\epsilon_k^\alpha$ through the exchange of $u_k \leftrightarrow v_k$, and

$$\delta\epsilon_k^\xi = J(\sqrt{2}q_2 - 2q_1) + O(S^{-1}).$$  

In Eqs. (62)-(64) above, the quantities $q_1$ and $q_2$ are defined by (thermodynamic limit)

$$
q_1 = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk (v_{k}^2), \quad q_2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk (\gamma_k u_k v_k).
$$

We remark that in deriving Eqs. (62)-(64), we have neglected terms containing anomalous products, such as, $\alpha_k^1 \beta_k^1$ and vertex corrections.

Lastly, the above results of our perturbative 1/$S$ series expansion lead to the effective Hamiltonian:

$$
\mathcal{H}^J_{eff} = E^J_{GS} - J N_c + \sum_k (\epsilon_k^\alpha \alpha_k + \epsilon_k^{(\beta)} \beta_k \beta_k + \epsilon_k^{(5)} \epsilon_k \epsilon_k),
$$

where

$$
E^J_{GS} = E_0 + E_1 + E_2,
$$

which can be read from Eqs. (52), (59), and (62), respectively, is the second-order result up to $O(1/S)$ for the GS energy, and

$$
\epsilon_k^{(s)} = \epsilon_k^0 + \delta_k^{(s)}, \quad \text{with } s = \alpha, \beta, \xi,
$$

are the corresponding second-order spin-wave modes, where the linear and the second-order correction terms are given by Eq. (60) and Eqs. (63)-(65), respectively.

A. Second-order spin-wave analysis

Our perturbative 1/$S$ series expansion approach is able to improve the LSWT result for the gap $\Delta = J$ of the antiferromagnetic mode, which should be compared with the second-order result derived from $\epsilon_k^{(\beta)}$, Eqs. (60), (63) and (68), at $k = 0$: $\Delta = (1 + \sqrt{2} q_2) J \approx 1.676 J$, in full agreement with similar spin-wave calculations for $AB_2$ [19] and spin-1/2-spin-1 [64, 65] chains, and in agreement with numerical estimates using exact diagonalization, $\Delta = 1.759 J$, for both $AB_2$ [5] and spin-1/2-spin-1 [63] chains. On the other hand, the LSWT predicts a gap $\Delta_{flat} = J$ for the flat ferromagnetic mode ($\epsilon_k^{(\xi)}$) in $AB_2$ chain, whereas our second-order spin-wave theory finds, using Eqs. (60), (64) and (68): $\Delta_{flat} = (1 - 2 q_1 + \sqrt{2} q_2) J \approx 0.66 J$, in full agreement with a similar spin-wave procedure [19]. Surprisingly, the estimated value from Exact Diagonalization (ED) [5]: $\Delta_{flat} = 1.0004 J$, lies between these two theoretical values. In fact, analytical approaches are still unable to reproduce the observed level crossing found in numerical calculations [5, 19] for the two ferromagnetic modes. This is probably due to the fact that the different symmetries exhibited by the localized excitation (flat mode) and the ferromagnetic dispersive mode are not explicitly manifested in the analytical approaches, so the levels avoid the crossing.

B. Ground state energy

In the thermodynamic limit, the second-order result for the GS energy of the $AB_2$ chain per unit cell reads:

$$
\frac{E^J_{GS}}{N_c} = -4JS^2 + \frac{J S}{2\pi} \int_{-\pi}^{\pi} dk \left( \sqrt{9 - 8\gamma_k^2} - 3 \right) - 2J(q_1^2 + q_2^2 - \frac{3}{\sqrt{2}} q_1 q_2).
$$

We remark that, at half filling, we shall not consider the constant term $-J N_c$ in Eq. (51), with the purpose of comparison with preceding results. Performing the integration over the first BZ and taking $S = 1/2$, we obtain that the GS energy per site at zero-field is given by $-0.4869 J$. This result agrees very well with values obtained using exact diagonalization [45] ($-0.485 J$) and DMRG [67] ($-0.4847 J$) techniques. For the spin-1/2 - spin-1 chain, the value obtained using DMRG [62] is $-0.72704 J$. To compare it with our finding, we need to multiply this value by $2/3$ (ratio between the number of sites of the two chains), yielding $-0.48469 J$.

C. Sublattice magnetizations and Lieb GS total spin per unit cell

In order to derive results beyond LSWT, we introduce staggered magnetic fields coupled to spins $S_{z}^L$ and $S_{z}^{B_i}$, with $l = 1, 2$, through the Zeeman terms: $-h_A \sum_i S_{z}^A + h_B \sum_i S_{z}^{B_i}$, which are added to $\mathcal{H}^J_{eff}$ in Eq. (47). Thus, $\langle \langle S_{z}^A \rangle \rangle$ and $\langle \langle S_{z}^{B_i} \rangle \rangle$ corresponding to sublattices $A$ and $B_i$ are obtained from $\langle \langle S_{z}^L \rangle \rangle = -1/N_c \sum_{i=1,2} [\langle \langle E_i(h_A) \rangle \rangle \langle \langle h_A \rangle \rangle]_{h_A=0}$, and an analogous equation for $\langle \langle S_{z}^{B_i} \rangle \rangle$ using Eqs. (59) and (62):

$$
\langle \langle S_{z}^A \rangle \rangle, \langle \langle S_{z}^{B_i} \rangle \rangle = \mp S \pm \left( \frac{1}{2} \frac{1}{4} \right) \frac{1}{\pi} \int_{-\pi}^{\pi} dk v_k^2 \left( \frac{1}{2} \frac{1}{4} \right) \frac{q_1}{\pi S} \int_{-\pi}^{\pi} dk \left( \frac{\gamma_k^2}{9 - 8\gamma_k^2} \right)^{3/2} + O(\frac{1}{S^2}).
$$

Carrying out the above integration, we obtain $\langle \langle S_{z}^A \rangle \rangle = -0.316343$ and $\langle \langle S_{z}^{B_i} \rangle \rangle = 0.408172$. These results are in good agreement with those obtained using DMRG [11] and ED [5] techniques: $\langle \langle S_{z}^A \rangle \rangle = -0.2925$ and $\langle \langle S_{z}^{B_i} \rangle \rangle = 0.3962$, respectively, and with values for $\langle \langle S_{z}^A \rangle \rangle$ and $\langle \langle S_{z}^{B_i} \rangle \rangle$ for the spin-1/2 - spin-1 chain [62–65]. Although at zero temperature, the sublattice magnetizations are strongly reduced by quantum fluctuations, as compared with their classical values, the unit cell magnetization remains $S_L \equiv 1/2$, where $S_L$ is the Lieb GS total spin per unit cell, in full agreement with Lieb’s theorem [5, 15] for bipartite lattices:

$$
S_L = \frac{1}{2} \| N_A - N_B \|,
$$

with $N_A(N_B)$ denoting the total number of spins in sublattice $A(B)$ per unit cell.
\[ \mathcal{H}_{\text{eff}}^{t-J} = - \sum_{i,\mu=a,d,e} \frac{\partial \mathcal{L}_{\text{eff}}}{\partial (\partial_{\nu_i} U_{i}^{(\mu)})}_{\sigma,\sigma} \left( \partial_{\nu_i} U_{i}^{(\mu)} \right)_{\sigma,\sigma} + \sum_{i,\nu_i} \frac{\partial \mathcal{L}_{\text{eff}}}{\partial (\partial_{\nu_i} U_{i}^{(\nu)})}_{\sigma,\sigma} \left( \partial_{\nu_i} U_{i}^{(\nu)} \right)_{\sigma,\sigma} + \mathcal{L}_{\text{eff}} \cdot T, \]

where

\[ \frac{\partial \mathcal{L}_{\text{eff}}}{\partial (\partial_{\nu_i} U_{i}^{(\mu)})}_{\sigma,\sigma} = \theta(-\sigma)(U_{i}^{(\mu)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i, \]

\[ \frac{\partial \mathcal{L}_{\text{eff}}}{\partial (\partial_{\nu_i} U_{i}^{(\nu)})}_{\sigma,\sigma} = \theta(\sigma) \left( U_{i}^{(\nu)} \right)_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i + \left( U_{i}^{(\nu)} \right)_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i. \]

From which we can write the effective t-J Hamiltonian as

\[ \mathcal{H}_{\text{eff}}^{t-J} = \mathcal{H}^t + \mathcal{H}^J, \]

where

\[ \mathcal{H}^t = -t \sum_{i,\sigma} \left\{ \theta(-\sigma)(U_{i}^{(b)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i + \theta(\sigma)(U_{i}^{(c)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i^\dagger + \theta(\sigma)(U_{i}^{(e)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i \right\} + \text{H.c.}, \]

and

\[ \mathcal{H}^J = -\frac{J}{4} \sum_{i,\mu=\nu} \theta(\sigma)(U_{i}^{(d)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i + \theta(\sigma)(U_{i}^{(e)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i + \frac{J}{4} \sum_{i,\mu=\nu} \theta(-\sigma)(U_{i}^{(d)})_{\sigma,\sigma} \alpha_i^{(1/2)} \alpha_i. \]

Notice that Eqs. (74) and (75) are identical to Eqs. (42c) and (42d), since Eqs. (42a) and (42b) were eliminated through the Legendre transformation.

Some digression on \( \mathcal{H}_{\text{eff}}^{t-J} \) is in order. One of the key properties of quasi-1D interacting quantum systems is the phenomenon of spin-charge separation, leading to the formation of spin and charge-density waves, which move independently and with different velocities. It has been demonstrated [24] that for \( \delta > 2/3 \) the low-energy physics of the doped \( AB_2 \) Hubbard chain in the \( U = \infty \) coupling limit is described in terms of the Luttinger-liquid model, with the spin and charge degrees of freedom decoupled. Most importantly, it has been shown that for the \( AB_2 \) t-J Hubbard chains [25] charge and spin quantum fluctuations are practically decoupled, as suggested by the emergence of charge-density waves in anti-phase with the modulation of the ferrimagnetic order. One can make use of this feature to formally split each term of the t-J Hamiltonian, Eq. (73)-(75), into a product of two independent terms acting on different Hilbert spaces, i.e., we can enforce spin-charge separation and calculate the charge and spin correlation functions in a decoupled fashion.

Therefore, from the above discussion, we shall consider that the charge correlation functions are well described by an effective spinless tight-binding model [24, 55, 68], since the hole (charge) density waves develop along the \( x \)-axis and in anti-phase with the modulation of the ferrimagnetic structure, as numerically observed in Fig. 2(b) of Ref. [25]. So, using Eqs. (33), with \( a/2 \rightarrow a \) (effective lattice spacing of the linear chain: distance between \( A \) and \( B \) sites, see Fig. 2(a) of Ref. [25]), we find

\[ \langle \alpha_i^{(1/2)} \alpha_i \rangle = \frac{1}{N_c} \sum_{k \neq 0} e^{-ik(x_i-1)} e^{ikx_i} \langle \Psi_0 \left| \alpha_i \alpha_k \right| \Psi_0 \rangle = \frac{1}{\pi} \int_{-k_F(\delta)}^{k_F(\delta)} e^{ik} dk = \frac{2}{\pi} \sin[k_F(\delta)], \]

with \( \langle \Psi_0 \rangle \) being the hole-doped ferrimagnetic GS, where \( k_F(\delta) = \pi N_c \equiv \pi \delta \) is the Fermi wave vector of the spinless tight-binding holes. In the same fashion: \( \langle \alpha_i^{(1/2)} \alpha_i^{\dagger} \rangle = \frac{2}{\pi} \sin[k_F(\delta)] \) and \( \langle \alpha_i \rangle = \langle \alpha_i \rangle^\dagger = 0 \); while \( \langle \sigma_i \rangle = \langle \alpha_i \rangle = \langle \alpha_i \rangle^\dagger = 0 \). Here, we remark that the itinerant holes away from half filling are associated with the lower-energy dispersive \( \alpha_k \) and \( \alpha_k^{\dagger} \) bands [see Fig. 1(b) in Sec. (II)], thus contributing to the kinetic Hamiltonian in Eq. (74). On the other hand, the local correlations related to the lower-energy bands \( \alpha_k \) and \( \alpha_k^{\dagger} \) contribute equally to the exchange Hamiltonian in Eq. (75). Thereby, using the above tight-binding results for the charge correlation functions, \( \mathcal{H}_{\text{eff}}^{t-J} \) in Eqs. (73)-(75) gives rise to the \( \delta \)-dependent Hamiltonian, \( \mathcal{H}_{\text{eff}}^{t-J}(\delta) = \mathcal{H}_{\text{eff}}^t(\delta) + \mathcal{H}_{\text{eff}}^J(\delta) \), written below:

\[ \mathcal{H}_{\text{eff}}^{t-J}(\delta) = -\frac{2}{\pi} \sin[k_F(\delta)] \sum_{i} \left( (U_{i}^{(b)})_{\sigma,\sigma} (U_{i}^{(d)})_{\sigma,\sigma} \right)_{\nu_i} + \left( (U_{i}^{(b)})_{\sigma,\sigma} (U_{i}^{(d)})_{\sigma,\sigma} \right)_{\nu_i} + \text{H.c.} \]

where the sum over \( \sigma \) was evaluated in Eq. (74) and the square of the \( SU(2) \) gauge field products in the exchange contribution have been summed up in Eq. (75), so that this contribution is just \( (1 - \delta) \) times \( \mathcal{H}_{\text{eff}}^{t-J} \) at half filling, Eq. (45), or alternatively, in terms of spin fields, Eq. (47), or spin-waves, Eqs. (66)-(68). On the other hand, the \( SU(2) \) gauge fields ma-
where $E_{AB}(65)$, the total GS energy (no spin-wave excitations) per unit cell in the thermodynamic limit is readily obtained: although the flat mode is strongly affected by the presence of holes, it remains dispersionless. In addition, using Eqs. (80) and $\epsilon_{\alpha}$ and $\epsilon_{\beta}$ are first-neighbor sites, and the flux quantum $\phi_0 = \hbar c/e \equiv 1$. If one consider that the carrier is at the site $iA$, we have four hopping possibilities: $iA \rightarrow iB_{1,2}$ and $iA \rightarrow (i + 1)B_{1,2}$, so the total phase $\phi$ acquired by the carrier in this prescription satisfies Stokes’ theorem: $\phi = \oint_{\text{unit cell}} A \cdot dA = \oint_{S} h \cdot dS = \hbar a^2 (a \equiv 1)$. We also remark that, in order to obtain real values for the zero-field staggered magnetizations, we have considered, for convenience, an imaginary gauge transformation $[56, 70]: A \rightarrow iA$. Therefore, by placing Eq. (78) and the similar matrix element into the kinetic term in Eq. (77), making the above Peierls substitution, and using the Holstein-Primakoff and Bogoliubov transformations introduced in Eqs. (48)-(50) and Eqs. (56)-(57), respectively, up to order $O(S^{-1})$, we arrive at the following diagonalized kinetic Hamiltonian $H^t_{eff}(\delta, h)$:

$$H^t_{eff}(\delta, h) = -\frac{4\sqrt{2}}{\pi} t e^{-(h_A + h_{B_1} + h_{B_2})} \sin[k_F(\delta)] \sum_{k} (4S - 3v_k^2 - (u_k^2 + 2v_k^2)\alpha_k^1 \alpha_k + (2u_k^2 + v_k^2)\beta_k^1 \beta_k - \xi_k^1 \xi_k),$$

where the doped-induced contributions for the spin dispersion relations are evidenced in the last three terms. On the other hand, by adding the Zeeman terms (see Sec. IV C) to the exchange contribution $H^J_{eff}(\delta)$, given in Eq. (77), we obtain $H^J_{eff}(\delta, h)$. Lastly, by adding the kinetic and the exchange contributions, we arrive at the effective $t$-$J$ Hamiltonian in the presence of a magnetic field:

$$H^J_{eff}(\delta, h) = -\frac{4\sqrt{2}}{\pi} t e^{-(h_A + h_{B_1} + h_{B_2})} \sin[k_F(\delta)] \sum_{k} (4S - 3v_k^2) + J(1 - \delta)(E^J_{GS} - JN_c) + \sum_{k} \epsilon^{(\alpha)}(\delta)\alpha_k^1 \alpha_k + \epsilon^{(\beta)}(\delta)\beta_k^1 \beta_k + \epsilon^{(\xi)}(\delta)\xi_k^1 \xi_k - h_A \sum_{i} S_i^{A,z} - h_{B_1} \sum_{i} S_i^{B_1,z} - h_{B_2} \sum_{i} S_i^{B_2,z},$$

where $E^J_{GS}$ is given by Eq. (67) and (69), and the corresponding spin-wave modes [see Eqs. (79), (60), (63)-(65), and (68)] of the doped $AB_2$ $t$-$J$ chain read:

$$\epsilon^{(\alpha)}(\delta) = \frac{4\sqrt{2}}{\pi} t \sin(\pi \delta)[u_k^2 + 2v_k^2] + (1 - \delta)(\epsilon^{(0)}_k + \delta \epsilon^{(\alpha)}_k),$$

$$\epsilon^{(\beta)}(\delta)$$ is obtained from $\epsilon^{(\alpha)}(\delta)$ through the exchange $u_k \leftrightarrow v_k$ and the replacement $\alpha \rightarrow \beta$, while

$$\epsilon^{(\xi)}(\delta) = \frac{4\sqrt{2}}{\pi} t \sin(\pi \delta) + (1 - \delta)(\epsilon^{(0)}_k + \delta \epsilon^{(\xi)}_k).$$

We find it instructive to comment on the analytical structure of the above equations. Firstly, we mention the presence of the Bogoliubov parameters [see Eqs. (57)] in a symmetric form in the kinetic terms of Eq. (81) and its analogous for $\epsilon^{(\beta)}(\delta)$; besides, although the flat mode is strongly affected by the presence of holes, it remains dispersionless. In addition, using Eqs. (80) and (65), the total GS energy (no spin-wave excitations) per unit cell in the thermodynamic limit is readily obtained:

$$E^J_{GS}(\delta, h)/N_c = -\frac{4\sqrt{2}}{\pi} t e^{-(h_A + h_{B_1} + h_{B_2})} \sin(\pi \delta)(4S - 3q_1) + (1 - \delta)(E^J_{GS}/N_c - J) - \sum_{l=1,2} S^{A,z}_l h_A - \sum_{l=1,2} S^{B_l,z} h_{B_l},$$

where $\sum_{l=1,2} S^{A,z}_l h_A$ and $\sum_{l=1,2} S^{B_l,z} h_{B_l}$ represent the total GS energy (no spin-wave excitations) per unit cell in the thermodynamic limit is readily obtained:
where \( \langle S^A,z \rangle \) and \( \langle S^B,z \rangle \) are the calculated sublattice magnetizations, at half filling and zero-field, given by Eqs. (70).

In subsections V A, V B, and V C, we will show that the underlying competing physical mechanisms: the magnetic orbital response and the Zeeman contribution embedded in Eqs. (80)-(83) will dramatically affect the behavior of the system under hole doping and, in particular, will lead to spiral IC spin structures, the breakdown of the spiral ferrimagnetic GS at a critical value of the hole doping, a region of phase separation, and RVB states at \( \delta \approx 1/3 \).

### A. Doped regime: Spin-wave modes

Before we go one step further to discuss relevant macroscopic quantities, i.e., the GS energy and total spin in the doped regime, we shall first undertake a detailed study, at a microscopic level, of the hole-doping effect on the calculated spin-wave branches given by Eqs. (81)-(82).

Fig. 2 depicts the second-order spin-wave dispersion relations at \( J/t = 0.3 \) and for the indicated values of \( \delta \). Without loss of generality, we set \( t = 1 \) in our numerical computations. At half filling, the antiferromagnetic mode \( \epsilon_k^{(\beta)} \), together with the two ferromagnetic modes: the dispersive \( \epsilon_k^{(\alpha)} \) and the flat one \( \epsilon_k^{(\gamma)} \), are shown in Fig. 2(a), which are defined in Eq. (68), and can be plotted using Eqs. (60) and (63)-(65).

As the hole doping increases slightly, the abrupt decrease of the peaks at \( k = 0 \) and \( k = \pi \) of the numerical DMRG structure factor (see Fig. 3 of Ref. [25]), associated with the ferrimagnetic order, manifests itself here through the opening of a gap in the ferromagnetic Goldstone mode \( \epsilon_k^{(\alpha)} \), as seen in Fig. 2(b), thus indicating that the system loses its long-range order. Note that the antiferromagnetic mode \( \epsilon_k^{(\beta)} \) is also similarly shifted. On the other hand, although the dispersion relation is modified for small values of the wave vector \( k \), the minimum value of \( \epsilon_k^{(\alpha)} \) still remains at \( k = 0 \) up to the onset of the formation of spiral IC spin structures at \( \delta_c(\text{IC}) = 0.043 \) (a value that should be compared with the numerical DMRG estimate of \( \delta \approx 0.055 \pm 0.012 \)), characterized by the flattening of the dispersive spin-wave branches around zero. Upon further increase of \( \delta \), two minima form (around \( k = 0 \)) and move away from each other as one enhances the hole doping. This behavior is the signature of the occurrence of spiral IC spin structures (see Fig. 3 of Ref. [25]).

Fig. 2(c) shows the onset of phase separation (PS) at \( \delta(\text{PS}) = 0.165 \) for \( J = 0.3 \), which is characterized by the overlap of the two ferromagnetic modes at \( k = 0 \). The signature of this regime is the spatial coexistence of two phases: spiral IC spin structures at \( \delta(\text{PS}) = 0.165 \) and RVB states at \( \delta \approx 1/3 \). In very good agreement with the numerical estimate of \( \delta_{\text{IC-PS}} \approx 0.16 \) [25]. At \( \delta \approx 1/3 \), the flat mode has the lowest energy, as illustrated in Fig. 2(d). This behavior indicates that the RVB state is the stable phase at \( \delta \approx 1/3 \) and \( J = 0.3 \) [25], and also in agreement with the numerical DMRG studies [11, 24] and analytical prediction at \( U = \infty \) [55].

In order to better understand the rich variety of doping-induced phases in the system, in Fig. 3 we plot the evolution of the wave vector \( \delta_{\text{min}} \) corresponding to the local minimum of \( \epsilon_k^{(\alpha)}(\delta) \), upon increasing the hole doping \( \delta \) from 0 to 1/3. The wave vector \( \delta_{\text{min}} \) remains zero until it hits the onset doping value \( \delta_{\text{IC}}(\text{IC}) = 0.043 \), beyond which a square-root growth behavior takes place [71]: \( |\delta - \delta_{\text{IC}}(\text{IC})|^{1/2} \) (blue line), for \( \delta \) close to \( \delta_{\text{IC}}(\text{IC}) \). The square-root growth behavior is the signature of the occurrence of a second-order quantum phase transition from the doped ferrimagnetic phase to the IC spiral ferrimagnetic state with a non-zero value of the total GS spin, \( S_{\text{GS}} \). This result is supported by the behavior of \( \Delta_{\delta} \equiv \delta_{\text{max}} - \pi \) at which the local maximum of the numeric DMRG structure factor \( S(k) \) near \( k = \pi \) is observed, as shown in the inset of Fig. 3 (taken from the inset of Fig. 3(b) of Ref. [25]). For further increase of hole doping our result deviates from the square-root growth behavior and some very interesting features are to be noticed. The value of \( \delta_c = 0.08 \) indicates the breakdown of the total \( S_{\text{GS}} \) in the IC phase, as will be confirmed by the explicit calculation of \( S_{\text{GS}} \), a macroscopic quantity, in Section V C. Thus, for \( 0.08 < \delta < 0.165 \) the system displays an IC phase with zero \( S_{\text{GS}} \), in agreement with the DMRG data (see Fig. 1(c) of Ref. [25]). At \( \delta(\text{PS}) = 0.165 \).
the system exhibits a first-order transition accompanied by the
spatial phase separation regime: the IC phase with zero \( S_{GS} \)
and modulation fixed by \( \delta(PS) \) in coexistence with the short-
range RVB states at \( \delta \approx 1/3 \), also consistent with the DMRG
data plotted in Fig. 4 of Ref. [25].

Lastly, we emphasize that, despite the occurrence of several
doping-induced phases in the DMRG studies [25]: Lieb ferri-
magnetism, spiral IC spin structures, RVB states with finite
spin gap, phase separation, and Luttinger-liquid behavior, it is
surprising and very interesting that the second-order spin-
wave modes remain stable up to \( \delta \approx 1/3 \), with predictions
in very good agreement with the DMRG studies [25]. In this
context, it is worth mentioning the long time studied case of
rare earth metals [72], where an external magnetic field can in-
duce non-trivial phase transitions involving spiral spin struc-
tures, well described by spin-wave theory.

B. Doped regime: Ground state energy

Performing the integration over the first BZ in Eqs. (65) and
(69) and setting \( S = 1/2 \) in Eq. (83), we find that the \( AB_2 t-J \)
ground state energy per unit cell as a function of hole doping
in zero-field reads:

\[
E_{GS}^{t-J}(\delta)/JN_c = -1.9543 \frac{t}{J} \sin(\pi\delta) - 2.4608 (1 - \delta). \quad (84)
\]

We shall now examine the case of small hole doping away
from half filling, i.e., with hole concentration ranging from
\( \delta = 0 \) up to \( \delta = 0.2 \) for two values of \( J: 0.1 \) and \( 0.3 \). In
Fig. 4, we show the evolution of the GS energy per unit cell
of the \( AB_2 t-J \) model as a function of hole doping for both
mentioned values of \( J \), and the comparison was made with the
numerical DMRG data [25]. From the two results at \( J = 0.3 \),
the only quantitative difference induced by the increase of the
hole concentration is a crossing feature around \( \delta \approx 0.1 \), where
our analytical result slightly change its behavior by lowering
the energy with respect to the numerical data [25]. In fact,
because our model assumes a ferrimagnetic state as the starting
point, this change of behavior suggests that we have entered in
a region of strong magnetic instabilities, and possibly indicat-
ing a smooth transition to an incommensurate phase with zero
GS total spin beyond \( \delta \approx 0.1 \), as confirmed by the numerical
data in Ref. [25] and illustrated in Fig. 3. On the other hand,
at \( J = 0.1 \), although our results reproduce the numerical data
with an acceptable agreement, we observe a discrepancy that
increases with \( \delta \). The cause of such discrepancy will be dis-
credited in the next subsection.

With the purpose of determining the interplay between the
contribution of magnetic exchange and the itinerant kinetic
energy to the zero-field GS energy Eq. (83), we take \( J = 0.3 \)
and show its evolution with doping in Fig. 5. We can see in
the insets, Fig. 5(a) and Fig. 5(b), the competitive behavior
of the two energetic contributions, i.e., the contribution of
the exchange energy increases linearly with \( \delta \), while a prac-
tically linear decrease of the hopping term is observed as one
enhances the hole doping. This competition indicates that a
phase transition to a paramagnetic phase should occur at some
critical concentration value.

C. Doped regime: Ground state total spin

The existence of a transition from an IC spiral ferrimag-
netic phase to an IC paramagnetic one is a most interest-
where the Nagaoka phenomenon is not manifested, that is, at \( J = 0.3 \), as indicated in Fig. 3. In this regime, spin and charge quantum fluctuations destabilize the ferrimagnetic structure and trigger a transition to an incommensurate paramagnetic phase at \( \delta_c \), with \( S_{GS} \sim (\delta - \delta_c) \rightarrow 0 \).

VI. CONCLUSIONS

In summary, we have presented a detailed analytical study of the large-U Hubbard model on the quasi-one-dimensional \( AB_2 \) chain. We used a functional integral approach combined with a perturbative expansion in the strong-coupling regime that allowed us to properly analyze the referred system at and away from half filling.

At half filling, our model was mapped onto the quantum Heisenberg model, and analyzed through a spin-wave perturbative series expansion in powers of \( 1/S \). We have demonstrated that the GS energy, spin-wave modes, and sublattice magnetizations are in very good agreement with previous results. In the challenging hole doping regime away from half filling, the corresponding \( t-J(= 4t^2/U) \) Hamiltonian was derived. Further, under the assumption that charge and spin quantum correlations are decoupled, the evolution of the second-order spin-wave modes in the doped regime has unveiled the occurrence of spatially modulated spin structures and the emergence of phase separation (first-order transition) in the presence of resonating-valence-bond states. The doping-dependent GS energy and total spin per unit cell are

...
also calculated, in which case the collapse of the spiral magnetic order at a critical hole concentration was observed. Remarkably, our above-mentioned analytical results in the doped regime are in very good agreement with density matrix renormalization group studies, where our assumption of spin-charge decoupling is numerically supported by the formation of charge-density waves in anti-phase with the modulation of the ferrimagnetic structure.

Finally, we stress that our reported results evidenced that the present approach, also used in a study on the compatibility between numerical and analytical outcomes of the large-U Hubbard model on the honeycomb lattice, was proved suitable for the $AB_2$ chain (a quasi-1D system), where the impact of charge and spin quantum fluctuations are expected to manifest in a stronger way. We thus conclude that our approach offers a quite powerful analytical description of hole-doping induced phases away from half filling in low-dimensional strongly-correlated electron systems.

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