# Ground-state separability and criticality in interacting many-particle systems

Federico Petrovich<sup>1</sup>, N. Canosa<sup>1</sup>, and R. Rossignoli<sup>1,2</sup>

<sup>1</sup>Instituto de Física de La Plata, CONICET, and Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, C.C. 67, La Plata (1900), Argentina <sup>2</sup>Comisión de Investigaciones Científicas (CIC), La Plata (1900), Argentina

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We analyze exact ground state (GS) separability in general *N*-particle systems with two-site couplings. General necessary and sufficient conditions for full separability in the form of one- and two-site eigenvalue equations are first derived. The formalism is then applied to a class of SU(n)-type interacting systems where each constituent has access to *n*-local levels, and where the total number parity of each level is preserved. Explicit factorization conditions for parity-breaking GSs are obtained, which generalize those for *XYZ* spin systems and correspond to a fundamental GS multilevel parity transition where the lowest  $2^{n-1}$  energy levels cross. We also identify a multicritical factorization point with exceptional high degeneracy proportional to  $N^{n-1}$ , arising when the total occupation number of each level is preserved, in which *any* uniform product state is an exact GS. Critical entanglement properties (such as full range pairwise entanglement) are shown to emerge in the immediate vicinity of factorization. Illustrative examples are provided.

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# I. INTRODUCTION

The ground state (GS) of strongly interacting spin systems, whereas normally entangled [1-3], can exhibit the remarkable phenomenon of factorization when a suitable magnetic field is applied [4-12]. This means that for such a field, the spin system admits a completely separable exact GS, i.e., a product of single spin states, despite the presence of nonnegligible couplings between the spins and the finite value of the applied field. Moreover, such a product state is not necessarily trivial, in the sense that it may break fundamental symmetries of the Hamiltonian. In this case, factorization signals in finite systems a special critical point where two or more levels with definite symmetry cross and the GS becomes degenerate [9–11,13,14], allowing for such symmetry-breaking exact eigenstates. The exact GS then typically undergoes in this case a transition between states with distinct symmetry as the factorization point is traversed, leading to visible effects in system observables [9,10,13,14]. Furthermore, critical entanglement properties emerge in the immediate vicinity [7,9,10,13,14], stemming ultimately from the product nature of the closely lying eigenstate.

Most studies of GS factorization have so far been restricted to interacting spin systems (see also Refs. [15–18]), where factorization conditions remain analytically manageable due to the small number of parameters required to specify an individual spin state. The main aim of this paper is to investigate exact GS factorization in more general interacting systems, i.e., beyond the standard SU(2) spin scenario, where already the characterization of a single component state is more complex. With this goal, we first derive the necessary and sufficient conditions for factorization in the form of eigenvalue equations, either for effective pair Hamiltonians or for the mean-field (MF) Hamiltonian and residual couplings.

We then apply the formalism to a general N-component interacting system in which each constituent has *n* accessible local levels such that the Hamiltonian can be expressed in terms of operators satisfying an U(n) algebra. For n = 2 it reduces to a general anisotropic XYZ spin system [19] in an applied transverse field [4,6,10,18], sharing with the latter the basic level number parity symmetry. For full range couplings it comprises schematic SU(n) models employed in nuclear physics for describing collective excitations [20-22], while for first neighbor couplings and special choices of parameters it reduces to the SU(n) Heisenberg model also known as the Uimin-Lai-Sutherland model [23-25]. The study of interacting many-body systems with global SU(n) symmetry has aroused great interest in recent years, becoming an active research topic that links the fields of condensedmatter and atomic, molecular, and optical physics [26-31]. Systems possessing high-dimensional symmetry can unveil exotic many-body physics and are suitable for describing a wide range of nontrivial phenomena. The paradigmatic SU(n) Heisenberg model [23–25], first employed in solidstate physics in connection with the integer quantum Hall effect [32,33], played also an important role in identifying unconventional magnetic states and phases [28,34-41]. Interest on the subject has been stimulated by the unprecedented advances in quantum control techniques, which offer the possibility of realizing strongly interacting many-body systems with high symmetry in alkaline-earth atomic gases in optical lattices [27,28,31]. These platforms have also received attention in relation with high-precision atomic clocks [42] and quantum computation [43].

The general factorization formalism is presented in Sec. II, whereas its application to a general SU(n)-type model for N components is described in Sec. III. Explicit equations for the existence of uniform parity-breaking factorized GSs are determined and shown to correspond to a multilevel parity transition occurring for any size N and coupling range where the GS becomes  $2^{n-1}$ -fold degenerate (if  $N \ge n-1$ ). A critical factorization point with exceptionally high degeneracy (which increases with size N) is also identified in systems with full level number symmetry, where any uniform separable state is an exact GS. Entanglement properties in the vicinity of factorization together with signatures of factorization in small systems are as well discussed. Conclusions are drawn in Sec. IV. Appendices discuss further details including the MF approximation in the model, which admits an analytic solution in the uniform case for arbitrary n.

### **II. FORMALISM**

# A. General factorization conditions

We consider a system described by a Hilbert space  $\mathcal{H} = \bigotimes_{p=1}^{N} \mathcal{H}_p$  such that it can be seen as a composite of N subsystems with Hilbert spaces  $\mathcal{H}_p$ . In this scenario we assume a general Hamiltonian containing one-site terms  $h_p$  plus two-site interactions  $V_{pq}$ ,

$$H = \sum_{p} h_{p} + \frac{1}{2} \sum_{p \neq q} V_{pq},$$
 (1)

$$h_{p} = \sum_{\mu} b_{\mu}^{p} o_{p}^{\mu}, \quad V_{pq} = \sum_{\mu,\nu} J_{\mu\nu}^{pq} o_{p}^{\mu} o_{q}^{\nu}, \quad (2)$$

where  $\{\sigma_p^{\mu}\}$  denotes a complete set of linearly independent operators over  $\mathcal{H}_p$  and  $J_{\mu\nu}^{pq} = J_{\nu\mu}^{qp}$  are the coupling strengths of the interaction between sites p and q. In particular, any spin array with two-spin interactions in a general applied magnetic field fits into this form. We use the notation  $\sigma_p^{\mu} \equiv$  $\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \sigma_p^{\mu} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$  when operators are applied to global states.

We are here interested in the conditions which ensure that a completely separable state,

$$|\Psi\rangle = \bigotimes_{p} |\psi_{p}\rangle = |\psi_{1}, \dots, \psi_{N}\rangle, \qquad (3)$$

possibly breaking some fundamental symmetry of H is an *exact* eigenstate of H,

$$H|\Psi\rangle = E|\Psi\rangle. \tag{4}$$

When applied to  $|\Psi\rangle$ , *H* can just connect it with itself and with superpositions of one- and two-site excitations,

$$|\Phi_p\rangle = |\psi_1, \dots, \phi_p, \dots, \psi_N\rangle, \tag{5}$$

$$|\Phi_{pq}\rangle = |\psi_1, \dots, \phi_p, \dots, \phi_q, \dots, \psi_N\rangle, \tag{6}$$

where  $\langle \phi_p | \psi_p \rangle = \langle \phi_q | \psi_q \rangle = 0$ . Then Eq. (4) implies the necessary and sufficient conditions,

$$\langle \Phi_p | H | \Psi \rangle = 0, \quad p = 1, \dots, N,$$
 (7)

$$\langle \Phi_{pq} | H | \Psi \rangle = 0, \quad 1 \leqslant p < q \leqslant N, \tag{8}$$

to be satisfied  $\forall |\phi_p\rangle$ ,  $|\phi_q\rangle$  orthogonal to  $|\psi_p\rangle$ ,  $|\psi_q\rangle$ , respectively. Since,

$$\langle \Phi_p | H | \Psi \rangle = \langle \phi_p | \tilde{h}_p | \psi_p \rangle, \quad \tilde{h}_p = h_p + \sum_{q \neq p} v_p^{(q)}, \quad (9)$$

where  $\tilde{h}_p$  is the local MF Hamiltonian at site p and

$$v_p^{(q)} = \langle \psi_q | V_{pq} | \psi_q \rangle = \sum_{\mu,\nu} J_{\mu\nu}^{pq} \langle o_q^{\nu} \rangle o_p^{\mu}, \tag{10}$$

the average potential at p due to the coupling with site q  $(\langle o_q^v \rangle = \langle \psi_q | o_q^v | \psi_q \rangle)$ , Eqs. (7) imply  $\langle \phi_p | \tilde{h}_p | \psi_p \rangle = 0 \ \forall | \phi_p \rangle$  orthogonal to  $| \psi_p \rangle$  and, hence, the eigenvalue equations,

$$\tilde{h}_p |\psi_p\rangle = \lambda_p |\psi_p\rangle, \quad p = 1, \dots, N.$$
(11)

As expected, each local state  $|\psi_p\rangle$  in  $|\Psi\rangle$  should be an eigenstate of the local MF Hamiltonian  $\tilde{h}_p$  determined by the same  $|\Psi\rangle$ , implying self-consistency.

It is now convenient to rewrite H as

$$H = \sum_{p} \tilde{h}_{p} + \frac{1}{2} \sum_{p \neq q} \tilde{V}_{pq}, \qquad (12)$$

where  $\tilde{V}_{pq} = V_{pq} - v_p^{(q)} - v_q^{(p)}$  is a residual coupling satisfying  $\langle \Phi_p | \tilde{V}_{pq} | \Psi \rangle = \langle \Phi_q | \tilde{V}_{pq} | \Psi \rangle = 0$ . Then,

$$\langle \Phi_{pq} | H | \Psi \rangle = \langle \phi_p, \phi_q | \tilde{V}_{pq} | \psi_p, \psi_q \rangle, \tag{13}$$

and Eqs. (8) together with previous property imply that  $|\Psi\rangle$  should be an eigenstate of all  $\tilde{V}_{pq}$ ,

$$\tilde{V}_{pq}|\psi_p,\psi_q\rangle = \lambda_{pq}|\psi_p,\psi_q\rangle, \quad 1 \le p < q \le N,$$
(14)

with  $\lambda_{pq} = \langle \tilde{V}_{pq} \rangle = -\langle V_{pq} \rangle$ . As  $\lambda_p = \langle h_p \rangle + \sum_{q \neq p} \langle V_{pq} \rangle$ , the total energy verifies  $E = \sum_p \lambda_p + \frac{1}{2} \sum_{p \neq q} \lambda_{pq} = \langle H \rangle$ . Therefore, we can state the following theorem:

The product state  $|\Psi\rangle$  is an exact eigenstate of the Hamiltonian (1) iff  $|\Psi\rangle$  is a simultaneous eigenstate of all one-site

*MF* Hamiltonians  $\bar{h}_p$  and all residual couplings  $\bar{V}_{pq}$ . Once Eqs. (11) and (14) are fulfilled, additional single-site terms having  $|\psi_p\rangle$  as GS  $(\Delta h_p |\psi_p\rangle = \Delta \lambda_p |\psi_p\rangle)$  can be added to *H* without affecting the product eigenstate. They can be used to remove the eventual degeneracy and bring down its energy  $(E \rightarrow E + \sum_p \Delta \lambda_p)$ , making it a nondegenerate GS for sufficiently large  $\Delta \lambda_p < 0 \forall p$ .

### B. Pair equations and the uniform case

Equations (11) and (14) imply that *H* can be written as a sum of pair Hamiltonians  $H_{pq} = H_{qp}$  ( $p \neq q$ ) having the pair product state  $|\psi_p, \psi_q\rangle$  as eigenstate,

$$H = \frac{1}{2} \sum_{p \neq q} H_{pq}, \qquad (15)$$

$$H_{pq}|\psi_p,\psi_q\rangle = E_{pq}|\psi_p,\psi_q\rangle, \quad 1 \le p < q \le N.$$
(16)

For instance, we can set  $H_{pq} = r_{pq}(\tilde{h}_p + \tilde{h}_q) + \tilde{V}_{pq}$  with  $r_{pq} = r_{qp}$  numbers satisfying  $\sum_q r_{pq} = 1 \forall p \text{ (and } r_{pp} = 0)$  in which case  $E_{pq} = r_{pq}(\lambda_p + \lambda_q) + \lambda_{pq}$ . The converse is trivially true: Eqs. (15) and (16) imply Eq. (4) for state (3) with

$$E = \frac{1}{2} \sum_{p \neq q} E_{pq}.$$
 (17)

Moreover, if  $|\psi_p, \psi_q\rangle$  is a GS of  $H_{pq} \forall p \neq q$ ,  $|\Psi\rangle$  will clearly be *a* GS of *H* since it will minimize *each average*  $\langle H_{pq}\rangle$  in (15), and, hence, the full average  $\langle H\rangle$ .

The pair Hamiltonians will have the general form

$$H_{pq} = h_p^{(q)} + h_q^{(p)} + V_{pq}, ag{18}$$

with  $\sum_{q \neq p} h_p^{(q)} = h_p$ . Then, when multiplied by  $\langle \psi_q |$ , Eq. (16) leads to  $(h_p^{(q)} + v_p^{(q)}) | \psi_p \rangle = \lambda_p^{(q)} | \psi_p \rangle$  with  $\lambda_p^{(q)} = E_{pq} - \langle h_q^{(p)} \rangle$ , implying Eq. (11) when summed over q (with  $\lambda_p = \sum_q \lambda_p^{(q)}$ ) and also Eq. (14) (with  $\lambda_{pq} = E_{pq} - \lambda_q^{(p)} - \lambda_p^{(q)})$ . Equations (15)–(16) and (11)–(14) are then equivalent.

By expanding the local states  $|\psi_p\rangle$  in an orthogonal basis  $|\psi_p\rangle = \sum_i f_i^p |i_p\rangle$  with  $f_i^p = \langle i_p |\psi_p\rangle$ ,  $\sum_i |f_i^p|^2 = 1$ , Eq. (16) becomes, explicitly,

$$\sum_{j,l} \left[ \delta_{kl} \langle i_p | h_p^{(q)} | j_p \rangle + \delta_{ij} \langle k_q | h_q^{(p)} | l_q \rangle + \langle i_p k_q | V_{pq} | j_p l_q \rangle \right] f_j^p f_l^q$$
  
=  $E_{pq} f_i^p f_k^q$ , (19)

to be fulfilled  $\forall$ , *i*, *k*. For dim  $\mathcal{H}_{p(q)} = n_{p(q)} \ge 2$  and general couplings, Eq. (19) imposes  $m = n_p n_q - 1$  complex equations to be satisfied by product states  $|\psi_p, \psi_q\rangle$  having  $l = n_p + n_q - 2 < m$  free complex parameters  $f_i^p$ ,  $f_j^q$ , hence, entailing restrictions on the feasible coupling strengths  $J_{\mu\nu}^{pq}$  and fields  $b_{\mu}^p$ . Factorization will then take place at special "points" or "curves" in parameter space. In particular, If  $H_{pq}$  is real in the previous pair product basis, one could always satisfy (19) by adjusting the diagonal elements  $\langle i_p k_q | V_{pq} | i_p k_q \rangle$ .

A simple realization of Eqs. (15) and (16) is the case of a uniform system where all local Hilbert spaces  $\mathcal{H}_p$  and operators  $\sigma_p^{\mu}$  are identical, whereas couplings between sites are all proportional (or zero) such that  $J_{\mu\nu}^{pq} = r_{pq}J_{\mu\nu}$  and

$$V_{pq} = r_{pq}V, \quad V = \sum_{\mu,\nu} J_{\mu\nu} o^{\mu} \otimes o^{\nu}, \tag{20}$$

$$h_{p}^{(q)} = r_{pq}h, \quad h = \sum_{\mu} b_{\mu}o^{\mu},$$
 (21)

in (18), with *V* and *h* independent of *p* and *q* (and  $J_{\mu\nu} = J_{\nu\mu}$ ). Here  $r_{pq} = r_{qp}$  determines the relative strength of the coupling between *p* and *q* and, hence, the range of the interaction. Eqs. (20) and (21) imply

$$h_p = r_p h, \quad r_p = \sum_{q \neq p} r_{pq}, \tag{22}$$

$$H_{pq} = r_{pq}(h \otimes \mathbb{1} + \mathbb{1} \otimes h + V), \qquad (23)$$

such that all  $H_{pq}$  become proportional.

Then a *uniform product eigenstate* with  $|\psi_p\rangle = |\psi\rangle \forall p$  may become feasible for special couplings as *all* pair equations (16) reduce in this case to the *single* equation,

$$(h \otimes \mathbb{1} + \mathbb{1} \otimes h + V)|\psi,\psi\rangle = E_2|\psi,\psi\rangle, \qquad (24)$$

after setting  $E_{pq} = r_{pq}E_2$ . The total energy (17) becomes

$$E = \frac{1}{2} E_2 \sum_{p} r_p.$$
 (25)

Here  $E_2$  represents a common pair energy whereas  $r_p$  a sort of coordination number for site p. In uniform cyclic systems  $r_p$ 

is constant  $\forall p$  and  $E = r_p \frac{N}{2} E_2$ , whereas in open systems  $r_p$  is typically smaller at the borders due to the smaller number of coupled neighbors, entailing edge corrections in  $h_p = r_p h$ . We will normalize the factors  $r_{pq}$  such that  $r_p = 1$  for inner "bulk" sites (e.g.,  $r_{pq} = \frac{1}{2} \delta_{p,q\pm 1}$  for first-neighbor couplings in a linear chain,  $r_{pq} = \frac{1}{N-1}$  for fully and equally connected systems).

### C. Formulation for fermion and boson systems

Previous equations admit a second quantized formulation for systems of fermions or bosons. For *N* of such particles at *N* distinct (orthogonal) sites labeled by *p*, having each  $n_p = \dim \mathcal{H}_p$  accessible local states labeled by *i*, we can define the corresponding creation and annihilation operators  $c_{pi}^{\dagger}$ ,  $c_{pi}$  satisfying

$$[c_{pi}, c_{qj}^{\dagger}]_{\pm} = \delta_{pq}\delta_{ij}, \quad [c_{pi}^{\dagger}, c_{qj}^{\dagger}]_{\pm} = [c_{pi}, c_{qj}]_{\pm} = 0 \quad (26)$$

for fermions (+) or bosons (-) ( $[a, b]_{\pm} = ab \pm ba$ ). Setting  $o_p^{\mu} = g_p^{ij} = |i_p\rangle\langle j_p|$  and replacing it with  $c_{pi}^{\dagger}c_{pj}$ , we can express the equivalent of Hamiltonian (1) as

$$H = \sum_{p,i,j} b_{ij}^{p} c_{pi}^{\dagger} c_{pj} + \frac{1}{2} \sum_{p \neq q} \sum_{i,j,k,l} J_{ijkl}^{pq} c_{pi}^{\dagger} c_{qk}^{\dagger} c_{ql} c_{pj}, \qquad (27)$$

with  $b_{ij}^p = \bar{b}_{ji}^p$ ,  $J_{ijkl}^{pq} = J_{klij}^{qp}$ , and  $J_{ijkl}^{pq} = \bar{J}_{jilk}^{pq}$  for *H* Hermitian. It preserves the total occupancy at each site,

$$[H, N_p] = 0, \quad N_p = \sum_{i} c_{pi}^{\dagger} c_{pi}, \tag{28}$$

(where  $[a, b] = [a, b]_{-}$ ). We will consider the single occupancy sector  $N_p = 1 \forall p$  where the formulation in the previous form (1) is equivalent. The commutators,

$$[c_{pi}^{\dagger}c_{pj}, c_{qk}^{\dagger}c_{ql}] = \delta_{pq}(\delta_{jk}c_{pi}^{\dagger}c_{pl} - \delta_{il}c_{pk}^{\dagger}c_{pj})$$
(29)

are the same for fermions and bosons and are identical to those satisfied by  $g_p^{ij} = |i_p\rangle\langle j_p| ([g_p^{ij}, g_q^{kl}] = \delta_{pq}(\delta_{jk}g_p^{il} - \delta_{il}g_p^{kj}))$ , defining an U( $n_p$ ) algebra at each site.

The product state (3) corresponds in the fermionic or bosonic scenario to an independent particle state,

$$|\Psi\rangle = \left(\prod_{p} a_{p1}^{\dagger}\right)|0\rangle, \quad a_{pj}^{\dagger} = \sum_{i} U_{ji}^{p} c_{pi}^{\dagger}, \qquad (30)$$

where  $U_{ji}^{p}$ 's are the elements of a unitary matrix  $U^{p}$  such that the same relations (26) are fulfilled by the new operators  $a_{pj}^{\dagger}$ ,  $a_{pi}$ . Then the one- and two-site excitations (7) and (8) can be written as

$$|\Phi_{p}\rangle = a_{pi}^{\dagger}a_{p1}|\Psi\rangle, \quad |\Phi_{pq}\rangle = a_{pi}^{\dagger}a_{q1}^{\dagger}a_{q1}a_{p1}|\Psi\rangle \tag{31}$$

for  $|\phi_p\rangle = a_{pi}^{\dagger}|0\rangle$ ,  $|\phi_q\rangle = a_{qj}^{\dagger}|0\rangle$ , and  $i, j \ge 2$ . Thus, we can employ expression (19) with  $f_i^p = U_{1i}^p$  and

$$\langle i_p k_q | V_{pq} | j_p l_q \rangle = J_{ijkl}^{pq}.$$
(32)

# **III. APPLICATION TO** *n***-LEVEL MODELS**

We will now consider the problem of factorization in a general n-level model with two-site interactions. It can be formulated as a system of N particles at N-distinct sites p,

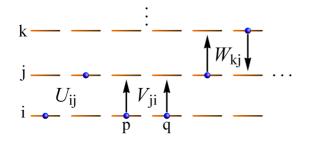


FIG. 1. Schematic diagram of the U, V, and W couplings in the Hamiltonian (33).

having each access to *n*-local levels with unperturbed energies  $\epsilon_i^p$ . The Hamiltonian reads

$$H = \sum_{i,p} \epsilon_{i}^{p} c_{pi}^{\dagger} c_{pi} - \frac{1}{2} \sum_{p \neq q} r_{pq} \sum_{i,j} (U_{ij} c_{pi}^{\dagger} c_{qj}^{\dagger} c_{qj} c_{pi} + V_{ij} c_{pi}^{\dagger} c_{qj}^{\dagger} c_{qj} c_{pj} + W_{ij} c_{pi}^{\dagger} c_{qj}^{\dagger} c_{qi} c_{pj}), \qquad (33)$$

where  $U_{ij} = U_{ji}$ ,  $V_{ij} = V_{ji}$ , and  $W_{ij} = W_{ji}$  are real coupling strengths and  $r_{pq} = r_{qp}$  determines the coupling range. The  $V_{ij}$  terms promote two particles at sites p, q from level j to i, whereas the  $W_{ij}$  terms interchange the occupancies of these levels at these sites (Fig. 1). For i = j both are identical to the  $U_{ii}$  term so we set  $V_{ii} = W_{ii} = 0$  in what follows. The  $U_{ij}$ terms just favor joint occupancy of levels i, j at sites p, q. The operators  $c_{ni}^{\dagger}c_{pj}$  satisfy an U(n) algebra at each site [Eq. (29)].

As discussed in Appendix A, for full range couplings  $(r_{pq} = \frac{1}{N-1} \forall p \neq q)$  the present model comprises the fully connected SU(*n*) fermionic nuclear models employed in Refs. [20–22], which are a *n*-level generalization of the well-known two-level Lipkin model [44,45]. Some SU(*n*) spin models and magnets [38,46,47] also correspond to special cases of (33), with the SU(*n*) invariant Heisenberg coupling [23–25,29,39,40] recovered for  $V_{ij} = U_{ij} = 0$  ( $i \neq j$ ) and  $W_{ij} = U_{ii} = J$ . In its distinguishable formulation, (33) is an *n*-level extension of the anisotropic *XYZ* spin-1/2 Hamiltonian in an applied magnetic field [4,6,10,14,48], recovered from (33) for n = 2. Besides, for n = 2s + 1 Eq. (33) can be formulated as a system of spins *s* with couplings depending on powers of the spin operators (see Appendix A).

Since particles are moved in pairs between levels, the Hamiltonian (33) has, for any value of the coupling strengths and range, the *number parity symmetries*,

$$[H, P_i] = 0, \quad i = 1, \dots, n, \tag{34}$$

$$P_i = \exp[-i\pi N_i], \quad N_i = \sum_p c^{\dagger}_{pi} c_{pi}, \quad (35)$$

where  $P_i$  is the parity of the total occupation  $N_i$  of level *i*. Since  $\prod_{i=1}^{n} P_i = e^{-i\pi N}$  is fixed, just n - 1 parities are independent. The exact eigenstates of *H* will then have definite parities when nondegenerate and can be characterized by their n - 1 values  $\sigma_i = \pm 1$  for i = 2, ..., n.

In the MF approximation, which in the uniform attractive case can be determined analytically (see Appendix B), the GS of (33) will typically exhibit a series of transitions as the coupling strengths increase from 0, from the unperturbed phase with all particles in the lowest i = 1 level to a final full

parity-breaking phase where all *n* levels are occupied, with intermediate steps where just m < n levels are nonempty. These transitions become smoothed out in the actual entangled exact GS for finite *N*, which may instead exhibit number parity transitions (Secs. III B and III E). The parity-breaking MF GS becomes, however, *exact* at the factorization point, discussed below.

# A. Uniform factorized GS

We now determine the conditions for which the Hamiltonian (33) possesses a uniform factorized GS,

$$|\Psi\rangle = \prod_{p} a_{p1}^{\dagger}|0\rangle, \quad a_{p1}^{\dagger} = \sum_{i} f_{i}c_{pi}^{\dagger}, \quad (36)$$

with  $f_i p$ -independent and  $\sum_i |f_i|^2 = 1$ . We set  $\epsilon_i^p = r_p \epsilon_i$  with  $r_p = \sum_{q \neq p} r_{pq}$  according to (22) such that factorization is determined by the single Eq. (24).

It is then seen that for k = i, Eq. (19) leads here to

$$\sum_{j} [(2\epsilon_i - U_{ii})\delta_{ij} - V_{ij}]f_j^2 = E_2 f_i^2,$$
(37a)

for i = 1, ..., n, which is a *standard eigenvalue equation* for the vector  $f^2$  of elements  $f_i^2$  (i.e., for the "squared wave function") and matrix  $M_{ij} = (2\epsilon_i - U_{ij})\delta_{ij} - V_{ij}$ ,

$$Mf^2 = E_2 f^2. \tag{37b}$$

It represents the  $n \times n$  *ii*-*jj* block in (19).

On the other hand, for  $k = j \neq i$ , Eq. (19) leads here to the  $2 \times 2 i j$ -ji block,

$$\begin{pmatrix} \epsilon_i + \epsilon_j - U_{ij} & -W_{ij} \\ -W_{ij} & \epsilon_i + \epsilon_j - U_{ij} \end{pmatrix} \begin{pmatrix} f_i f_j \\ f_j f_i \end{pmatrix} = E_2 \begin{pmatrix} f_i f_j \\ f_j f_i \end{pmatrix}.$$
 (38)

Equation (38) entails for  $f_i f_j \neq 0$  the constraint,

$$U_{ij} + W_{ij} = \epsilon_i + \epsilon_j - E_2. \tag{39}$$

Hence, given an arbitrary single-site spectrum  $\epsilon_i$  and couplings  $V_{ij}$ ,  $U_{ii}$ , the factorized eigenstate and pair energy  $E_2$  are first determined from the eigenvalue Eq. (37b). The couplings  $W_{ij}$  or  $U_{ij}$  for which such a state becomes an *exact* eigenstate are then obtained from (39). These conditions are *independent* of coupling range  $r_{pq}$  and system size N, implying that this factorization will emerge for any  $N \ge 2$  and range  $r_{pq}$  if (39) is satisfied. The total energy is determined by  $E_2$  through Eq. (25).

For *GS factorization*, the *lowest* eigenvalue  $E_2$  of (37) should be chosen. In this case, as the eigenvalues of the matrix in (38) are  $\epsilon_i + \epsilon_j - U_{ij} \mp W_{ij}$ , i.e.,  $E_2$  and  $E_2 + 2W_{ij}$  when (39) is fulfilled, the uniform factorized state will be a GS of the full pair Hamiltonian (and, hence, of the full *H*) for any signs of the  $V_{ij}$ 's if

$$W_{ij} \ge 0 \quad \forall i \neq j, \tag{40}$$

i.e.,  $E_2 \leq \epsilon_i + \epsilon_j - U_{ij} \forall i \neq j$ . Since the lowest eigenvalue of (37) satisfies  $E_2 \leq \text{Min}_i[2\epsilon_i - U_{ii}] \leq 2\epsilon_i - U_{ii} \forall i$ , a sufficient condition for the validity of (40) at fixed  $U_{ij}$  is

$$U_{ij} \leq (U_{ii} + U_{jj})/2,$$
 (41)

 $\forall i \neq j$ . In particular, (40) will be always satisfied for the lowest eigenvalue  $E_2$  if  $U_{ij} = 0 \forall i, j$  and (39) is fulfilled.

The factorized GS obtained from (37) coincides, of course, with the MF GS for the couplings (39), lying *within* the full parity-breaking MF phase (see Appendix B).

For n = 2, the factorization conditions (37), (39) reduce to those for the *XYZ* spin Hamiltonian (see Appendix A), leading to a factorizing field. And for n = 3 it is still possible to satisfy (39) by adjusting just the one-site energies  $\epsilon_i$  for given values of  $U_{ij}$  and  $W_{ij}$ ,

$$\epsilon_i = \frac{1}{2}(T_{ij} + T_{ik} - T_{jk} + E_2), \tag{42}$$

where T = U + W and  $i \neq j \neq k$ . In this case a constant diagonal term  $\Delta U_{ii} = U_0$  remains to be added in (37) in order that  $E_2$  matches the original value.

In the attractive case  $V_{ij} \ge 0 \forall i, j$ , the eigenvector  $f^2$  of (37) associated with the lowest eigenvalue  $E_2$  will have all components  $f_i^2$  of the same sign (in order to yield the lowest eigenvalue) and, hence, all  $f_i$  can be chosen as real. Otherwise some of the  $f_i^2$  can be negative, implying imaginary components  $f_i$ .

In systems that can be divided into even and odd sites such that any site p is coupled  $(r_{pq} \neq 0)$  just to sites q of opposite parity (such as first-neighbor couplings in a linear chain or cubic lattice), the uniform factorized GS can be used to generate, through local unitaries, *alternating* factorized GSs for associated Hamiltonians. For instance, if  $c_{pi}^{\dagger} \rightarrow -c_{pi}^{\dagger}$  for some level i at odd sites p, then  $V_{ij} \rightarrow -V_{ij}$ ,  $W_{ij} \rightarrow -W_{ij}$ , and  $|\Psi\rangle$  is changed into an alternating product GS  $|\Psi'\rangle$  with  $f_i^p \rightarrow (-1)^p f_i$ .

#### B. Parity breaking and degeneracy at factorization

Equations (37) just determine the squared coefficients  $f_i^2$ , leaving the sign of each  $f_i$  free. This degeneracy of the uniform factorized eigenstate (36) reflects its breaking of *all* number parity symmetries  $P_i$  if  $f_i \neq 0 \forall i$ : Its expansion in the standard product basis,

$$|\Psi\rangle = \sum_{i_1,\dots,i_N} f_{i_1}\cdots f_{i_N} c^{\dagger}_{1i_1}\cdots c^{\dagger}_{Ni_n} |0\rangle, \qquad (43)$$

clearly contains terms with all possible parities  $P_i$ . As

$$P_i c_{pi}^{\dagger} P_i^{\dagger} = -c_{pi}^{\dagger}, \qquad (44)$$

 $P_i|\Psi\rangle$  just changes the sign of  $f_i$ . Hence, if  $|\Psi\rangle$  is an exact eigenstate, all  $2^{n-1}$  parity transformed states,

$$|\Psi_{i_1\cdots i_m}\rangle = P_{i_1}\cdots P_{i_m}|\Psi\rangle \tag{45}$$

obtained by changing the signs of  $f_{i_1} \cdots f_{i_m}$  in (43) with  $m \leq n-1$ , are also exact eigenstates with the same energy due to (34). These parity-breaking product eigenstates can then only arise at a point where levels with different parities *cross and become degenerate*. Factorization then signals a *fundamental parity level crossing* taking place for *any* size *N* and range  $r_{pq}$  whenever Eq. (39) is fulfilled.

If  $N \ge n - 1$ , we obtain from (45)  $2^{n-1}$  nonorthogonal but linearly independent degenerate product eigenstates, implying a  $D = 2^{n-1}$  degeneracy at factorization, which indicates the number of distinct parity levels exactly crossing at this point.

On the other hand, for small systems with N < n - 1, the number D of linearly independent states obtained with such

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sign changes in the  $f_i$ , and, hence, the degeneracy at factorization is smaller. We obtain, in general,

$$D = \begin{cases} 2^{n-1}, & N \ge n-1\\ \sum_{k=0}^{N} {n-1 \choose k}, & N \le n-1, \end{cases}$$
(46)

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such that signs are to be changed in just  $k \leq N$  levels. For a single pair  $(N = 2), D = {n \choose 2} + 1$ .

We have so far assumed that the matrix M in (37) has a nondegenerate GS with a full rank eigenvector  $f^2$ . If  $f_i = 0$ for some *i*, then factorization (and the ensuing degeneracy) becomes equivalent to that for  $n \rightarrow n - 1$ . And if the GS of M is itself degenerate, the coefficients  $f_i^2$  will no longer be unique (after normalization). The GS of H will then exhibit additional degeneracy since a *continuous set* of factorized GSs becomes feasible. We will consider below a special extreme case.

# C. The W case: Number symmetry and exceptional degeneracy at factorization

We now consider the special case where  $V_{ij} = 0 \forall i \neq j$  in (33). For n = 2 it corresponds to the XXZ model (see Appendix A) which conserves the total  $S_z$  and, hence, has eigenstates with definite magnetization. Accordingly, for  $V_{ij} = 0$  Eq. (33) exhibits an additional symmetry: not only parity, but also the total occupation of each level is conserved

$$[H, N_i] = 0, \quad i = 1, \dots, n, \tag{47}$$

since the U and W couplings preserve all  $N_i$ 's. The exact eigenstates can then be characterized by the occupations  $N_i$  of each level, existing  $\frac{N!}{N_1!\cdots N_n!}$  orthogonal states with the same set of occupations  $(N_1, \dots, N_n)$ .

This higher symmetry entails, first, a trivial factorization: the n states with all particles in just one level,

$$|\Psi_i\rangle = \prod_p c_{pi}^{\dagger}|0\rangle, \quad i = 1, \dots, n$$
(48)

are clearly exact eigenstates:  $H|\Psi_i\rangle = E_i|\Psi_i\rangle$  with  $E_i = (\epsilon_i - \frac{1}{2}U_{ii})\sum_p r_p$ . For n = 2 they become the fully aligned spin states with maximum magnetization |M|.

But in addition, *nontrivial symmetry-breaking* uniform factorized eigenstates of the form (36) may also arise: Eqs. (37)–(39) remain valid, but Eq. (37) becomes trivial, implying, for a full rank solution with  $f_i \neq 0 \forall i$ ,

$$U_{ii} = 2\epsilon_i - E_2, \quad i = 1, \dots, n, \tag{49}$$

$$W_{ij} + U_{ij} = \epsilon_i + \epsilon_j - E_2 = \frac{U_{ii} + U_{jj}}{2}.$$
 (50)

Thus,  $f_i$  remains here *completely arbitrary*: For vanishing  $V_{ij}$  any uniform factorized state (36) is an exact eigenstate with the same energy (25) when (49)–(50) are fulfilled, as the matrix M becomes proportional to the identity. And if  $W_{ij} \ge 0 \forall i \ne j$ , i.e., if Eq. (41) holds  $\forall i \ne j$ , they will be *GSs* by the same previous arguments. The ensuing GS energy (25) is then *independent* of the number n of levels for a given fixed value of  $E_2$ .

Such a *continuous* set of factorized exact GSs reflects their breaking of *all* number symmetries (47) when  $0 < f_i < 1 \forall i$  as they lead to nonzero fluctuations  $\langle N_i^2 \rangle - \langle N_i \rangle^2 = N f_i (1 - 1)^2 = N f_i (1 - 1)^2$ 

 $f_i$ ) > 0. Moreover, since they contain terms with all possible values  $0 \le N_i \le N$  when  $f_i \ne 0 \forall i$ , all number projected states with definite values  $N_i = n_i \forall i$  derived from such product state  $|\Psi\rangle$ ,

$$|\Psi_{n_1\cdots n_n}\rangle \propto P_{n_1}\cdots P_{n_n}|\Psi\rangle,$$
 (51)

satisfying  $N_i |\Psi_{n_1 \cdots n_n}\rangle = n_i |\Psi_{n_1 \cdots n_n}\rangle$  with  $\sum_{i=1}^n n_i = N$ , will also be *exact eigenstates with the same energy* due to (47). Here  $P_{n_i} = \frac{1}{2\pi} \int_0^{2\pi} e^{-i\phi(N_i - n_i)} d\phi$  are number projectors  $([P_{n_i}, H] = 0 \forall i)$ .

Remarkably, when normalized these projected states become *independent* of the arbitrary coefficients  $f_i$  determining the product state  $|\Psi\rangle$  since each term in their expansion (43) will have exactly  $n_i$  particles in level *i* and, hence, all coefficients become identical:  $f_{i1} \cdots f_{i_N} = \prod_{i=1}^n (f_i)^{n_i} = C_{n_1 \cdots n_n}$ . Therefore, the states (51) become

$$\left|\Psi_{n_{1}\cdots n_{n}}\right\rangle = \left|n_{1}\cdots n_{n}\right\rangle,\tag{52}$$

where  $|n_1 \cdots n_n\rangle$  is the *fully symmetric* state having  $N_i = n_i$  particles in each level *i*. The total degeneracy at factorization is then given by the number of distinct projected states (52), which is just the number of ways of distributing *N* undistinguishable particles on *n* levels,

$$D = \binom{N+n-1}{n-1},\tag{53}$$

with  $D \approx \frac{N^{n-1}}{(n-1)!}$  for  $N \gg n$ . Then factorization arises at an *exceptional critical point where the D lowest levels with distinct values of the N<sub>i</sub>'s cross and become degenerate.* The ensuing degeneracy *grows* with system size, in contrast with previous *N*-independent parity degeneracy.

Since *any* uniform factorized state is an exact GS at the factorizing point, the GS subspace is here clearly *invariant under arbitrary* U(n) *unitary transformations*,

$$U = \exp\left[-i\sum_{i,j}T_{ij}\sum_{p}c_{pi}^{\dagger}c_{pj}\right],$$
 (54)

where T is an arbitrary Hermitian matrix, as U transforms any product state (36) into another uniform product state and these states span the GS subspace,

$$|\Psi\rangle \to U|\Psi\rangle \implies f \to \exp[-iT]f.$$
 (55)

It corresponds to  $U = e^{-iT} \otimes \cdots \otimes e^{-iT}$  in the distinguishable formulation.

The question which now arises is whether the full *H* also becomes SU(*n*) invariant when the factorizing conditions (49) and (50) are fulfilled. For n = 2 this is indeed the case: as shown in Appendix A, they lead to a Heisenberg Hamiltonian  $H \propto -\sum_{p < q} r_{pq} s_p \cdot s_q$  plus constant terms, where  $s_p$  is the (dimensionless) spin operator at site *p*. Such *H* is obviously invariant under arbitrary global rotations  $\exp(-i\phi k \cdot \sum_p s_p)$  with *k* an arbitrary unit vector, and admits any aligned product state  $|k, \ldots, k\rangle$  with  $\langle k | s_p | k \rangle = \frac{1}{2}k$  as exact GS for arbitrary *k*.

However, for  $n \ge 3$  only the GS subspace remains invariant, in general, i.e.,  $[H, U] \ne 0$ , with [H, U] having just D zero eigenvalues, corresponding to the GS subspace. Therefore, for  $n \ge 3$  the general SU(n) Heisenberg Hamiltonian

[23–25],

$$H = -J \sum_{p < q} r_{pq} \sum_{i,j} c^{\dagger}_{pi} c^{\dagger}_{qj} c_{qi} c_{pj}$$
(56)

is just a *particular case* of present factorizing Hamiltonian, corresponding to  $\epsilon_i = 0 \forall i$  and, hence,  $U_{ii} = J = -E_2 = W_{ij} \forall i \neq j$ , according to Eqs. (49) and (50).

## D. Definite parity eigenstates and entanglement at the border of factorization

We now examine the GS in the immediate vicinity of factorization. We consider first the  $V \neq 0$  case. Since away from factorization the exact GS is normally nondegenerate for finite *N*, it will have definite parities *P<sub>i</sub>*. The same holds for the other levels which meet at the factorization point. Therefore, their side limits at factorization will be given by the parity projected states,

$$\Psi_{\sigma_2\cdots\sigma_n}\rangle \propto (\mathbb{1} + \sigma_2 P_2)\cdots(\mathbb{1} + \sigma_n P_n)|\Psi\rangle, \qquad (57)$$

where  $\sigma_i = \pm 1$ , satisfying  $P_i | \Psi_{\sigma_2 \dots \sigma_n} \rangle = \sigma_i | \Psi_{\sigma_2 \dots \sigma_n} \rangle \forall i$ . This projection just selects from the expansion (43) those terms with the specified level parities. The GS will then exhibit a *parity transition* as the factorization point is crossed [9,10,14] (when some Hamiltonian parameter is varied), having distinct parities  $\sigma_i$  at each side.

These projected states are *entangled*, i.e., they are no longer product states. They exhibit critical entanglement properties since the product state  $|\Psi\rangle$  from which they are derived is uniform and has lost all information about the range  $r_{pq}$  of the coupling and the distance between sites. Accordingly, the exact side limits at factorization of GS entanglement entropies will be *range independent*. Moreover, pairwise entanglement will be independent of the separation |p - q| between sites, although it will remain small in compliance with monogamy [49,50].

These properties can be seen, for instance, in the reduced state of site p,  $\rho_p = \text{Tr}_{p' \neq p} |\Psi_0\rangle \langle \Psi_0 |$ , of elements,

$$(\rho_p)_{ij} = \langle c_{pj}^{\dagger} c_{pi} \rangle, \tag{58}$$

and eigenvalues  $\lambda_{pi}$ . Its entropy,

$$S_p = -\operatorname{Tr} \rho_p \log_2 \rho_p = -\sum_{i=1}^n \lambda_{pi} \log_2 \lambda_{pi}$$
(59)

is a measure of the (mode) entanglement between this site and remaining sites. In the fermion case it is also a measure of *fermionic* entanglement [45,51] in the sense of indicating the deviation of the state from an independent fermion state [Slater determinant (SD)], since it is the *p* block of the onebody density matrix  $\rho^{(1)}$ ,

$$\rho_{pi,qj}^{(1)} = \langle c_{qj}^{\dagger} c_{pi} \rangle = \delta_{pq} \langle c_{pj}^{\dagger} c_{pi} \rangle, \tag{60}$$

whose blocked structure is due to the fixed fermion number  $N_p$  at each site. Its entropy  $S(\rho^{(1)}) = \sum_p S_p$  is a quantity which vanishes iff  $|\Psi_0\rangle$  is a SD, i.e.,  $(\rho^{(1)})^2 = \rho^{(1)}$  [51,52], and is just  $NS_p$  in the uniform case. In the factorized state  $|\Psi\rangle$ ,  $\langle c_{pj}^{\dagger}c_{pi}\rangle = f_i^{p*}f_j^p$ , implying obviously  $\rho_p^2 = \rho_p$ , i.e.,  $\lambda_{pi} = \delta_{i1}$  as directly seen in the MF basis  $(\langle a_{pj}^{\dagger}a_{pi}\rangle = \delta_{ij}\delta_{i1})$ , and, hence,  $S_p = 0$ .

In contrast, in states  $|\Psi_0\rangle$  with definite parity all offdiagonal elements in the standard basis are canceled by parity conservation ( $[\rho_p, e^{i\pi c_{pi}^{\dagger} c_{pi}}] = 0 \forall i$ ), implying,

$$\langle c_{pi}^{\dagger} c_{pi} \rangle = \delta_{ij} \langle c_{pi}^{\dagger} c_{pi} \rangle. \tag{61}$$

Hence, the eigenvalues of  $\rho_p$  are just the average occupations  $\lambda_{pi} = \langle c_{pi}^{\dagger} c_{pi} \rangle$  and  $S_p > 0$  whenever  $\langle c_{pi}^{\dagger} c_{pi} \rangle \in (0, 1)$ .

In the projected states (57), these occupations depend on the parities  $\sigma_2, \ldots, \sigma_n$ . For instance, for n = 3 in the uniform case, we obtain for  $i = 1, \ldots, 3$ ,

$$\langle \Psi_{\sigma_2 \sigma_3} | c_{pi}^{\dagger} c_{pi} | \Psi_{\sigma_2 \sigma_3} \rangle$$

$$= |f_i|^2 \frac{1 + \sum_j (-1)^{\delta_{ij}} \sigma_j (1 - 2|f_j|^2)^{N-1}}{1 + \sum_j \sigma_j (1 - 2|f_j|^2)^N}, \qquad (62)$$

where  $\sigma_1 \sigma_2 \sigma_3 = (-1)^N$ . Hence, for large N,  $\lambda_{pi} \approx |f_i|^2$  plus corrections of order  $(1 - 2|f_j|^2)^{N-1}$ , which depend on the parities  $\sigma_j$ .

For finite *N* these corrections are, nonetheless, appreciable and their parity dependence originates the splitting of the degeneracy in the immediate vicinity of factorization (Appendix C). Moreover, the occupations (62) determine the *exact side limits* of the single-site entanglement entropy (59) at factorization, which will then remain *finite* at this point and exhibit a *discontinuity* due to the change in the GS parities  $\sigma_i$ . For large *N* this discontinuity becomes small as  $\lambda_{pi} \approx |f_i|^2$ approaches the MF value at both sides, but the side limits of  $S_p$  remain *finite*.

On the other hand, the entanglement between two sites  $p \neq q$  is determined by their reduced pair state  $\rho_{pq} = \text{Tr}_{p' \neq p,q} |\Psi_0\rangle \langle \Psi_0 |$ , also a mixed state. For general *n* it can be measured through the negativity [53–55],

$$\mathcal{N}_{pq} = \frac{1}{2} \big( \mathrm{Tr} \big| \rho_{pq}^{T_p} \big| - 1 \big), \tag{63}$$

where  $\rho_{pq}^{T_p}$  is the partial transpose of  $\rho_{pq}$ . Equation (63) is just minus the sum of the negative eigenvalues of  $\rho_{pq}^{T_p}$ , with  $\mathcal{N}_{pq} > 0$  ensuring entanglement of  $\rho_{pq}$  according to the Peres criterion [56]. The side limits at factorization of the exact GS negativities will be determined by the projected states (57) and will be *nonzero* for finite *N*, and, hence, *independent* of the separation between the sites and the coupling range for a uniform  $|\Psi\rangle$ , undergoing there a discontinuity due to the transition in the GS parities.

Although visible in small systems (see Sec. III E), the common value of  $\mathcal{N}_{pq}$  at factorization decreases as N increases, in agreement with monogamy: The projected states (57) involve a sum over  $2^{n-1}$  product states  $\sigma_{i_1}P_{i_1}\cdots\sigma_{i_m}P_{i_m}|\Psi\rangle$  having the signs of  $f_i$  changed at levels  $i_1, \ldots, i_m$ , which for sufficiently large N become approximately orthogonal (e.g., for n = 3 their overlaps are proportional to terms  $(1 - 2|f_j|^2)^N$ as seen in (62), which decrease rapidly with N if  $|f_j| \neq 0$ or 1. Neglecting these overlaps, the two-site reduced states  $\rho_{pq}$  derived from (57) become essentially a convex mixture of  $2^{n-1}$  product states  $\rho_p \otimes \rho_q$  and are then *separable* [56], implying  $\mathcal{N}_{pq} \approx 0 \forall p, q$ . Thus, for large systems pairwise entanglement vanishes at factorization, although it will still show long range in its vicinity [7,10,14]. We remark, however, that the exact GS side limits at factorization of other entanglement measures do remain finite for large *N* as was seen for the single-site entropy (59). In fact, previous argument entails that the reduced state  $\rho_M \equiv \rho_{p_1\cdots p_M}$  of M < N sites derived from (57) will be mixed with rank  $2^{n-1}$  (for  $M \ge n-1$ ) such that its entropy, measuring their entanglement with the rest of the system, will also have nonzero side limits for any *N*. They will be bounded, however, by this rank,

$$S(\rho_M) = -\operatorname{Tr} \rho_M \log_2 \rho_M \leqslant n - 1, \tag{64}$$

at the border of factorization. This bound at this point is then another signature of factorization in these systems.

Similar considerations hold for the V = 0 case. The level number projected states (51)–(52) represent the exact side limits at factorization of the *D* crossing states. Except for the states (48) with just one level occupied, all remaining states are entangled and lead again to critical entanglement properties (independence of coupling range and separation) due to their fully symmetric nature. In particular, they lead again to single-site reduced states  $\rho_p$  diagonal in the standard basis,

$$\langle n_1 \cdots n_n | c_{pi}^{\dagger} c_{p_i} | n_1 \cdots n_n \rangle = \delta_{ij} n_i / N, \qquad (65)$$

implying  $\lambda_{pi} = n_i/N$  and, hence, a single-site entropy  $S(\rho_p) > 0$  if  $1 \le n_i \le N - 1$  for some *i*.

# E. Factorization signatures in small systems

We discuss here typical illustrative results in small *n*-level systems. We examine first the case with both *V* and *W* couplings of Secs. III A and III B. We consider a uniform single-site spectrum  $\epsilon_i = \frac{\epsilon}{2}(i - \frac{n+1}{2})$  for i = 1, ..., n, and couplings  $U_{ij} = 0$ ,  $V_{ij} = v$ , and  $W_{ij} = (v/v_c)(\epsilon_i + \epsilon_j - E_{2c})$ , chosen such that GS factorization is reached at  $v = v_c$ , according to Eq. (39) ( $E_{2c}$  is the pair energy obtained from (37) at  $v = v_c$ ). For n = 2 these parameters lead to an anisotropic *XY* Heisenberg coupling in a uniform field [Eq. (A2) with  $J_z = 0$ ], whereas for general *n* it is an extension of the *n*-level model used in Refs. [21,22]. Figures 2–5 show results for the n = 3-level case with  $v_c = \frac{2}{5}\epsilon$  (for which  $E_{2c} \approx -1.26\epsilon$ ).

We first depict in Fig. 2 the spectrum of H for a single pair (N = 2,  $r_{12} = 1$ ) and for a cyclic four-particle chain with first-neighbor couplings (N = 4,  $r_{pq} = \frac{1}{2}\delta_{q,p\pm 1}$ ) as a function of  $v/v_c$ . In both cases there is a GS band of  $2^{n-1} = 4$  states which cross exactly at the factorization point  $v = v_c$  where a GS number parity transition takes place: The GS changes from the ( $\sigma_1, \sigma_2$ ) = (+, +) state for  $v < v_c$  to the ( $\sigma_1, \sigma_2$ ) = (-, -) state for  $v > v_c$ . These states form the border of the GS band, the remaining crossing levels ( $\sigma_1, \sigma_2$ ) = (±, ∓) lying in between.

Further results for a ring of N = 4 particles are shown in Fig. 3. It is verified that the first three exact excitation energies together with the difference with the mean-field (HF, see Appendix B) GS energy, exactly vanish just at  $v = v_c$ (top left), confirming factorization. The exact average occupations  $\langle n_i \rangle$  of each level are shown in the top-right panel (solid lines). As v increases the two upper levels start to be populated with all exact occupations undergoing a steplike discontinuity at the factorizing point, reflecting the associated

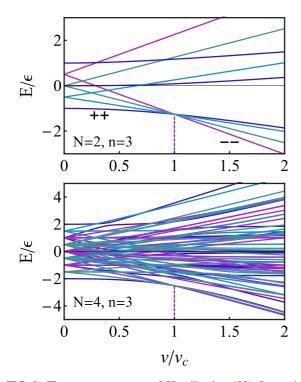


FIG. 2. The exact spectrum of Hamiltonian (33) for a single pair (N = 2, top) and for N = 4 sites (bottom) with first-neighbor couplings and n = 3 levels at each site as a function of the scaled coupling strength  $v/v_c$  (see text). In both cases factorization takes place at the same value  $v = v_c$  where Eqs. (37)–(39) are fulfilled and the four levels with distinct parities forming the GS band cross.

GS parity transition. The side limits at this point coincide with those determined by the projected states (57) through Eq. (62). Present factorization can then be detected and verified through the magnitude of these occupation jumps.

HF results reproduce qualitatively the general trend but miss the jump at factorization: Although exact at this point, the HF GS corresponds to a superposition of the crossing definite parity exact eigenstates. It exhibits instead transitions at  $v/v_c \approx 0.44$  and 0.65 ( $\forall N$ ) where the second and third level, respectively, start to be populated in the approach (see Appendix B) and parity symmetry becomes broken. Thus, factorization lies *within* the full parity-breaking HF phase (and not at a HF transition).

Entanglement properties are depicted in the lower panels. The exact single-site entanglement entropy (59) (bottom right) increases monotonously as  $v/v_c$  increases and displays a *step*-wise increase precisely at the factorizing point due to the transition in the average level occupations. The negativities  $\mathcal{N}_1$  and  $\mathcal{N}_2$  (bottom left), measuring the *pairwise* entanglement between first and second neighbors exhibit instead a stepwise *decrease* at factorization, indicating multipartite entanglement effects of the parity projected states. They are also verified to approach the *same side limits* at factorization, confirming the independence from separation in its immediate vicinity as predicted by the projected states (57).

In Fig. 4 we show the same quantities for a ring of N = 6 particles with the same parameters to view the trend for larger systems. Their behavior remains similar with factorization

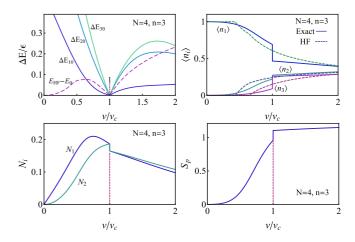


FIG. 3. Results for the N = 4 chain of Fig. 2. Top left: The first three exact excitation energies  $\Delta E_{i0} = E_i - E_0$  and the difference  $E_{\rm HF} - E_0$  with the Hartree-Fock (HF) GS energy. All vanish at the factorization point  $v = v_c$  (1). Top right: Exact (solid lines) and HF (dotted lines) values of the GS average occupations  $\langle n_i \rangle = \langle c_{pi}^{\dagger} c_{pi} \rangle$ of the three levels. The exact values represent the eigenvalues of the single-site reduced density matrix and exhibit a discontinuity at  $v = v_c$ . Bottom: The exact one-site entanglement entropy (59) (right), which shows a stepwise increase at factorization, and the exact negativities between first ( $\mathcal{N}_1 = \mathcal{N}_{p,p+1}$ ) and second ( $\mathcal{N}_2$ ) neighbors (left), measuring pairwise entanglement. Both reach the same side limits at factorization, exhibiting there a stepwise decrease.

located at the same point where the four lowest levels with distinct parities cross (top left). However, the GS now exhibits in the range considered two further parity transitions at  $v_{c2} \approx 1.52v_c$  and  $v_{c3} \approx 1.74v_c$ , not related to factorization, where just two levels cross and the GS parity changes from  $(\sigma_2, \sigma_3) = (+, +)$  for  $v < v_c$  to (-, -) for  $v_c < v < v_{c2}$ , (+, -) for  $v_{c2} < v < v_{c3}$  and back to (+, +) for  $v > v_{c3}$ .

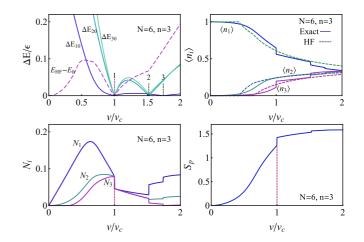


FIG. 4. Results for an N = 6 chain with n = 3 levels at each site. Details are similar to those of Fig. 3. Top left: The first three excitation energies  $\Delta E_{i0}$  together with  $E_{\rm HF} - E_0$ . Points 2 and 3 indicate other GS parity transitions. Top right: Exact and HF average occupations  $\langle n_i \rangle$ . Bottom: The one-site entanglement entropy (59) (right) and the exact negativities between first, second, and third  $(\mathcal{N}_3)$  neighbors (left). All  $\mathcal{N}_i$ 's reach the same side limits just at factorization ( $v = v_c$ ).

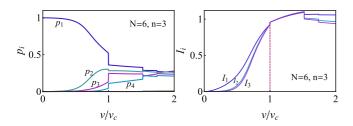


FIG. 5. The exact eigenvalues of the two-site reduced density matrix for first neighbors (left) and the mutual information  $I(\rho_{pq})$  for first  $(I_1)$ , second  $(I_2)$ , and third  $(I_3)$  neighbors (right) in the chain of Fig. 4. All  $I_i$ 's exactly merge at the side limits of the factorizing point  $v = v_c$ .

These transitions lead to further steps in the single-site occupation numbers and entropy (right panels), although the larger step occurs again at the factorizing transition. All three pair negativies  $N_i$  are verified to reach the *same side limits* at the factorizing point, a characteristic signature of uniform factorization, exhibiting there a stepwise decrease. These patterns are not repeated at the other GS parity transitions, where  $N_1$  increases but  $N_3$  decreases vanishing for  $v > v_{c3}$ . Full range pairwise entanglement is, thus, centered at the factorizing point where it becomes independent of separation. However, the side limits of N at factorization are smaller than for N = 4, in agreement with monogamy and previous considerations.

In Fig. 5 we show the eigenvalues  $p_i$  (entanglement spectrum) of the two-site density matrix  $\rho_{pq}$  (left panel), which determine the entanglement of the pair with the rest of the chain (just four of them are nonnegligible). They also exhibit steps at the parity transitions with the larger step again at the factorizing point. The ensuing mutual information,

$$I_{pq} = S(\rho_p) + S(\rho_q) - S(\rho_{pq}),$$
(66)

where  $S(\rho_p) = S_p$  is the single-site entropy is shown in the right panel for the first three neighbors. It is a measure of the total correlation between sites. It is seen that all three values merge at the side limits of the factorizing point, confirming again that in its vicinity correlations become independent of separation. Since it does not satisfy monogamy, its behavior is, however, different from that of the negativity, steadily increasing up to  $v_{c2}$  and exhibiting at factorization a stepwise increase.

Finally, Figs. 6 and 7 show the spectrum of *H* in the special *W* case ( $V_{ij} = 0$ ) of Sec. III C for N = 4 particles and cyclic first-neighbor couplings. In Fig. 6 we consider n = 3 (top) and 4 (bottom) levels at each site with uniform spectrum  $\epsilon_1 = -\epsilon$ ,  $\epsilon_2 = 0$ ,  $\epsilon_3 = 0.8\epsilon$  (and  $\epsilon_4 = 2.2\epsilon$  for n = 4), unequally spaced in order to avoid extra degeneracy away from factorization. We have set  $U_{ij} = \delta_{ij} \frac{w}{w_c} (2\epsilon_i - E_2)$  and  $W_{ij} = \frac{w}{w_c} (\epsilon_i + \epsilon_j - E_2)$  with  $w_c = \epsilon$  and  $E_2 = -5\epsilon$ , such that factorization takes place at  $w = w_c$  according to Eqs. (49) and (50) with GS energy  $\frac{N}{2}E_2 = -\frac{5}{2}N\epsilon$ , independent of *n*.

It is verified that all  $\binom{N+n-1}{N}$  levels (15 for n = 3 and 35 for n = 4) forming the GS band cross at the factorization point  $w = w_c$ , where any uniform product state is confirmed to be an exact GS. The side limits at  $w = w_c$  of the crossing states are the symmetric states (52) with definite occupations in all n levels, whose energies become all identical at this point, with

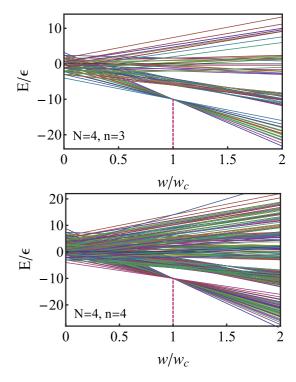


FIG. 6. The exact spectrum of Hamiltonian (33) for  $V_{ij} = 0$  and first-neighbor W and U couplings (see text) for N = 4 sites and n = 3 (top) and 4 (bottom) levels at each site, as a function of the scaled coupling strength  $w/w_c$ . Factorization arises at an exceptionally degenerate point  $w = w_c$  where 15 (35) levels cross for n = 3 (4), in agreement with Eq. (53). At this point *any* uniform factorized state is an exact GS.

the GS changing at  $w_c$  from  $|\Psi_1\rangle$  [Eq. (48), all particles in the first level] to  $|\Psi_n\rangle$  (all particles in the last level). No other multilevel crossing in higher excited states occurs at this point.

To complete the description, Fig. 7 depicts the spectrum for fixed couplings  $W_{ij} = U_{ii} = J > 0 \forall i, j$  and previous single-site energies as a function of the spacing  $\epsilon$  for n = 4levels. At fixed J factorization is then reached for  $\epsilon \rightarrow 0$ ,

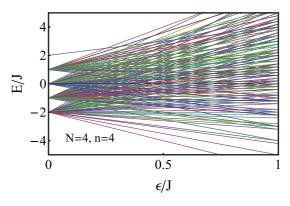


FIG. 7. The spectrum of Hamiltonian (33) for  $V_{ij} = 0$  and  $U_{ii} = W_{ij} = J \forall i, j$  as a function of the single-particle spacing  $\epsilon/J$  for N = n = 4 (see text). For  $\epsilon \rightarrow 0$  the SU(*n*) invariant Hamiltonian (56) is approached. In this limit any uniform factorized state is again an exact GS with the GS degeneracy (D = 35) given by the same Eq. (53).

where *H* becomes the SU(*n*) invariant Hamiltonian (56) and Eqs. (49) and (50) are fulfilled with  $E_2 = -J$  and GS energy  $-NJ/2 \forall n \ge 2$ . Again, all 35 levels of the initial GS band merge in this limit where any uniform product state becomes an exact GS.

However, in contrast with Fig. 6, it is seen that the remaining higher-energy levels also coalesce for  $\epsilon \rightarrow 0$  into four levels, three of them highly degenerate (the highest level remains nondegenerate) due the high symmetry of H for  $\epsilon = 0$ . Nevertheless, these higher-energy eigenspaces contain no fully factorized states. As can be seen from (49) and (50), even if nonuniform product states were considered, no further fully separable eigenstate is feasible for  $\epsilon = 0$ , apart from those of the GS subspace.

For N = 4 and  $n \ge 4$ , the spectrum of Hamiltonian (56) with first-neighbor couplings has just five distinct energies with uniform spacing:  $E_i = -J(3 - i)$  for i = 1, ..., 5. For n = 4 the level degeneracies are (35,110,60,50,1), the highest level corresponding to the fully antisymmetric eigenstate. We remark, however, that whereas the same factorized GSs hold *also* in the presence of long-range or nonuniform couplings, i.e., arbitrary  $r_{pq} > 0$  with the same degeneracy (53) (and the *same* energy if  $r_p = \sum_{q \neq p} r_{pq} = 1 \forall p$ ), the intermediate levels and degeneracies do depend on the coupling range and  $r_{pq}$  and are, hence, not "universal." Only the fully antisymmetric eigenstates, feasible for  $n \ge N$ , remain also unaltered with an energy which is just the opposite of that of the fully symmetric factorized eigenstates.

### **IV. CONCLUSIONS**

We have analyzed the problem of GS factorization beyond the standard interacting spin system scenario. We have first derived general necessary and sufficient factorization conditions for Hamiltonians with two-site couplings, showing that they can be recast as pair eigenvalue equations. These conditions were then applied to interacting N-particle systems where each constituent has access to n-local levels. For the UVW class of Hamiltonians (33) they can be worked out explicitly, leading in the uniform case to the eigenvalue equation (37) for the squared local wave function and the constraint (39) on the coupling strengths, valid for any number n of levels. They are independent of size N and coupling range and generalize those for XYZ spin systems, recovered for n = 2. The ensuing product state is shown to be a GS when conditions (40) are fulfilled, which are directly satisfied for vanishing  $U_{ij}$ .

The full rank factorized GS breaks all level number parities, preserved by the Hamiltonian, therefore, having a  $2^{n-1}$ degeneracy (for  $N \ge n-1$ ). Factorization then arises at a special point where all  $2^{n-1}$  definite parity levels of the GS band cross and become degenerate, signaling a fundamental GS level parity transition emerging for *any* size *N* and range.

We have also examined the special V = 0 case where the Hamiltonian preserves the total occupation of each level. Here the factorization conditions allowed us to identify an exceptional critical point, again emerging for any size and range where *all levels* with definite occupations  $N_i$  forming the GS band coalesce and become degenerate. This leads to a GS degeneracy which *increases with system size*  $(D \propto N^{n-1})$ . At

this point *all uniform product states*, including those breaking all occupation number symmetries, are exact degenerate GSs, implying a full SU(n) invariant GS subspace in a Hamiltonian which for  $n \ge 3$  is not necessarily SU(n) invariant.

Finally, we have analyzed the entanglement properties in the immediate vicinity of factorization. For small systems, pairwise entanglement (as detected by the negativity) reaches there full range and becomes *independent* of separation, thus, constituting an entanglement critical point. Moreover, in such systems the parity transition occurring at the factorizing point entails finite discontinuities in most quantities (single-site entanglement, negativity, level occupations, mutual information, etc.), whose magnitude can be analytically determined through projection of the factorized GS. On the other hand, for large systems pairwise entanglement will become vanishingly small at factorization for any pair, but long-range entanglement in its vicinity as well other effects [such as bounded values of block entropies, Eq. (64)] will remain visible.

To summarize, in addition to providing nontrivial analytic exact GSs in strongly coupled systems which are not exactly solvable (which could be used as benchmarks for approximate numerical techniques), symmetry-breaking factorization enables one to identify critical points in small samples with exceptional GS degeneracy and entanglement properties. Amid increasing quantum control capabilities, present results open the way to explore factorization in SU(n) many-body physics and complex systems beyond the usual SU(2) spin scenario.

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### APPENDIX A: SPECIAL CASES OF HAMILTONIAN (33)

We consider here particular cases of Hamiltonian (33). Fully connected fermionic U(n) nuclear models as those used in Refs. [20,21] correspond to  $r_{pq} = \frac{1}{N-1} \forall p \neq q$ . In this case, for  $U_{ij} = 0$  and  $\epsilon_i^p = \epsilon_i$  we can rewrite (33) as

$$H = \sum_{i=1}^{n} \epsilon_i G_{ii} - \frac{1}{2(N-1)} \sum_{i \neq j} V_{ij} G_{ij}^2 + W_{ij} (G_{ij} G_{ji} - G_{ii}),$$
(A1)

where  $G_{ij} = \sum_{p=1}^{\Omega} c_{pi}^{\dagger} c_{pj}$  are collective operators satisfying the same U(n) algebra as the operators  $g_{ij} = c_{ni}^{\dagger} c_{pj}$ ,

$$[G_{ij}, G_{kl}] = \delta_{jk}G_{il} - \delta_{il}G_{kj}$$

for both fermions and bosons. Equation (A1) is a simplified schematic model for describing collective excitations. For n = 2 and  $\epsilon_i = (-1)^i \epsilon/2$  it becomes the Lipkin Hamiltonian [44,45],

$$H = \epsilon S_z - \frac{1}{2(N-1)} [V(S_+^2 + S_-^2) + W(S_+S_- + S_-S_+ - N)],$$

where  $S_z = \frac{1}{2}(G_{22} - G_{11})$ ,  $S_+ = G_{21} = S_-^{\dagger}$  are collective spin operators satisfying the SU(2) algebra ( $[S_z, S_{\pm}] =$ 

 $\pm S_{\pm}$ ,  $[S_-, S_+] = 2S_z$ ) and  $V = V_{12}$ ,  $W = W_{12}$ . These models have been used to test several many-body techniques [21,22,44,45,57] as the exact eigenstates can be obtained by diagonalizing *H* in the irreducible representations of U(*n*). For n = 2 level number parity conservation reduces to the  $S_z$ -parity symmetry  $[H, P_z] = 0$ , where  $P_z = e^{-i\pi S_z} = P_2 e^{-i\pi N}$ .

On the other hand, in the distinguishable formulation, the Hamiltonian (33) corresponds for  $g_p^{ij} = |i_p\rangle\langle j_p|$  to

$$H = \sum_{i,p} \epsilon_{i}^{p} g_{p}^{ii} - \sum_{p < q, i, j} r_{pq} \left( U_{ij} g_{p}^{ij} g_{q}^{jj} + V_{ij} g_{p}^{ij} g_{q}^{ij} + W_{ij} g_{p}^{ij} g_{q}^{ji} \right)$$

For n = 2,  $\epsilon_i^p = (-1)^i b^p/2$ ,  $V_{12} = (J_x - J_y)/2$ ,  $W_{12} = (J_x + J_y)/2$ , and  $U_{11} = U_{22} = -U_{12} = J_z/2$  with p = 1, ..., N, it becomes the Hamiltonian of N spins 1/2 interacting through anisotropic XYZ couplings [6,10,19,48] of general range in a nonuniform field  $b^p$ ,

$$H = \sum_{p} b^{p} s_{pz} - \sum_{p \neq q} r_{pq} \sum_{\mu = x, y, z} J_{\mu} s_{p\mu} s_{q\mu}, \qquad (A2)$$

where  $s_{pz} = \frac{g_p^{22} - g_p^{11}}{2}$ ,  $s_{px} = \frac{g_p^{21} + g_p^{12}}{2}$ ,  $s_{py} = \frac{g_p^{21} - g_p^{12}}{2i}$  are spin operators satisfying the SU(2) algebra. For  $V_{12} = 0$  we recover the *XXZ* case where  $J_x = J_y$  and  $[H, S_z] = 0$ .

Besides, in the *n*-level case the operators  $g_p^{ij}$  can always be expressed in terms of powers of spin-s operators with 2s + 1 = n. For instance, for n = 3 all  $g_p^{ij}$  can be written in terms of spin-1 operators  $s_{pz}$  and  $s_{p\pm} = s_{px} \pm is_{py}$  as

$$g_p^{33} = \frac{1}{2} \left( s_{pz}^2 \pm s_{pz} \right), \quad g_p^{22} = \frac{1}{2} s_p^2 - s_{pz}^2,$$
 (A3)

$$g_p^{21} = -\frac{1}{\sqrt{2}} s_{p+} s_{pz}, \quad g_p^{32} = \frac{1}{\sqrt{2}} s_{pz} s_{p+},$$
 (A4)

with  $g_p^{31} = \frac{1}{2}s_{p+}^2$ ,  $g_p^{ji} = (g_p^{ij})^{\dagger}$ , and  $s_p^2 = s_{px}^2 + s_{py}^2 + s_{pz}^2 = 2\mathbb{1}_p$ . Thus, single-site operators become, in general, quadratic in the local spin components  $S_{p\mu}$ .

We now verify that for n = 2, factorization conditions (37)–(39) become those for the *XYZ* Hamiltonian in a uniform field  $b^p = b$  (A2). Equation (37a) leads for n = 2 to

$$E_2 = -J_z/2 - \sqrt{b^2 + V_{12}^2},$$

for the lowest pair energy with (39) implying  $W_{12} = -E_2 - U_{12}$ . We then obtain

$$|b| = \sqrt{(W_{12} - J_z)^2 - V_{12}^2} = \sqrt{(J_y - J_z)(J_x - J_z)},$$

which is the known expression for the factorizing field *b* at given couplings  $J_{\mu}$  [9,10] (valid for  $J_z < J_y < J_x$ , corresponding to  $W_{12} > 0$ ,  $V_{12} > 0$ ). Setting now  $f = (\cos \frac{\theta}{2}, \sin \frac{\theta}{2})$  for the local eigenvector Eq. (37a) leads to

$$\cos \theta = \frac{b - J_z/2 - E_2 - V_{12}}{b - J_z/2 - E_2 + V_{12}} = \sqrt{\frac{J_y - J_z}{J_x - J_z}},$$
 (A5)

which coincides with the known expression for the spin orientation angle  $\theta$  of the uniform product GS [9].

In the V = 0 case of Sec. III C, factorization Eqs. (49) and (50) imply  $U_{ii} = 2\epsilon_i - E_2$  and  $W_{12} = -E_2 - U_{12} \equiv J$  for n = 2 and  $\epsilon_2 = -\epsilon_1$ , leading to a Heisenberg Hamiltonian,

$$H = -\sum_{p \neq q} r_{pq} (J \boldsymbol{s}_p \cdot \boldsymbol{s}_q + C), \tag{A6}$$

with  $C = -\frac{1}{2}(E_2 + \frac{1}{2}J)$ . Both  $E_2$  and  $U_{12}$  are free parameters. It is verified that for J > 0, any uniform product state, i.e., any state with all spins aligned in a fixed direction  $\theta$ ,  $\phi$  [ $f = (\cos \frac{\theta}{2}, e^{i\phi} \sin \frac{\theta}{2})$ ] is an exact GS with pair energy  $E_2$  ( $s_p \cdot s_q | \psi, \psi \rangle = \frac{1}{4} | \psi, \psi \rangle$ ) and total energy (25).

# **APPENDIX B: MEAN-FIELD APPROXIMATION**

We show here that the MF approximation for the Hamiltonian (33) (which corresponds to the HF scheme in the fermionic case) can be solved analytically in the uniform attractive case for any values of n, N, and the coupling range  $r_{pq} \ge 0$ .

We look for the product state  $|\Psi\rangle$  [or, equivalently, the independent particle state (36)] which minimizes  $\langle H \rangle = \langle \Psi | H | \Psi \rangle$  with  $\epsilon_i^p = r_p \epsilon_i$  and nonegative couplings  $U_{ij}$ ,  $V_{ij}$ , and  $W_{ij}$ . As  $\langle c_{pi}^{\dagger} c_{qj} \rangle = \delta_{pq} f_i^{p*} f_j^p$  and  $\langle c_{pi}^{\dagger} c_{qi}^{\dagger} c_{ql} c_{pk} \rangle = f_i^{p*} f_j^{q*} f_k^p f_l^q$  for  $p \neq q$ , it is easily seen that in this case  $\langle H \rangle$  can be minimized by real uniform coefficients  $f_i^p = f_i \in \mathbb{R}$ . This leads, setting  $r = \sum_p r_p = \sum_{p \neq q} r_{pq}$ , to

$$\langle H \rangle = r \left( \sum_{i} \epsilon_{i} f_{i}^{2} - \frac{1}{2} \sum_{i,j} J_{ij} f_{i}^{2} f_{j}^{2} \right)$$
(B1)

$$= \frac{\prime}{2} \sum_{i,j} \tilde{M}_{ij} f_i^2 f_j^2, \quad \tilde{M}_{ij} = \epsilon_i + \epsilon_j - J_{ij}, \qquad (B2)$$

where  $J_{ij} = U_{ij} + V_{ij} + W_{ij}$  (and  $W_{ii} = V_{ii} = 0$ ). Thus, MF depends here just on the sum of coupling strengths.

In order to obtain the MF solution, we may directly minimize (B2) with respect to the  $f_i^2$  with the constraint  $\sum_i f_i^2 = 1$ . After introducing a Lagrange multiplier  $\lambda$ , this leads to the equation  $\sum_j \tilde{M}_{ij} f_j^2 = \lambda$  and, hence, to  $f_i^2 = \lambda \sum_j \tilde{M}_{ij}^{-1}$ , i.e.,  $f^2 = \lambda \tilde{M}^{-1} \boldsymbol{v}$  with  $\boldsymbol{v} = (1, ..., 1)^T$ . Enforcing the constraint leads to  $\lambda = 1/(\boldsymbol{v}^T \tilde{M}^{-1} \boldsymbol{v})$  and

$$\boldsymbol{f}^2 = \tilde{\boldsymbol{M}}^{-1} \boldsymbol{v} / (\boldsymbol{v}^T \tilde{\boldsymbol{M}}^{-1} \boldsymbol{v}). \tag{B3}$$

The minimum MF energy becomes

$$\langle H \rangle = \frac{r}{2} (\boldsymbol{f}^2)^T \tilde{\boldsymbol{M}} \boldsymbol{f}^2 = \frac{r}{2} (\boldsymbol{v}^T \tilde{\boldsymbol{M}}^{-1} \boldsymbol{v})^{-1} = \frac{r}{2} \lambda.$$
(B4)

Equations (B3) and (B4) provide a closed expression for the full parity breaking  $(f_i \neq 0 \forall i)$  MF state and energy. The sign of each  $f_i$  remains free, in agreement with parity breaking, entailing a  $2^{n-1}$  degeneracy of the MF state.

The exact factorized GS determined by Eqs. (37)–(39) is one of these solutions: At factorization, (39) implies  $J_{ij} = \epsilon_i + \epsilon_j - E_2 + V_{ij}$  for  $i \neq j$  and, hence,

$$\tilde{M}_{ij} = (2\epsilon_i - U_{ii})\delta_{ij} - (1 - \delta_{ij})(V_{ij} - E_2) = M_{ij} + E_2(1 - \delta_{ij}),$$
(B5)

with *M* the matrix in (37b). Equations (B3)–(B5) imply Eq. (37) with  $E_2 = (\mathbf{v}^T \tilde{M}^{-1} \mathbf{v})^{-1} = \lambda$  as the MF pair energy.

The restriction  $f_i^2 > 0 \forall i$  implies, however, a limit on the validity of solution (B3). The border is obtained from the condition  $f_i = 0$  for some *i* (normally the highest-energy level). Beyond this border we should set  $f_i = 0$ , obtaining a new MF solution with n - 1 occupied levels, given by (B3) with  $\tilde{M}$ , *v* restricted to the occupied levels. This solution

is valid until one of the new coefficients  $f_i^2$  vanishes. For decreasing coupling strengths, this is to be repeated until the trivial solution  $f_i = \delta_{i1}$  (valid for sufficiently small  $J_{ij}$ ) is reached.

Therefore, as  $J_{ij}$  increases from 0, a series of n-1 MF transitions normally arise, associated with the onset of occupation of the *i*th level. For instance, for  $U_{ii} = 0$  and  $J_{ij} = J(1 - \delta_{ij}), J > 0$ , Eq. (B3) leads to

$$f_i^2 = 1/n - \tilde{\epsilon}_i/J, \quad i = 1, ..., n,$$
 (B6)

where  $\tilde{\epsilon}_i = \epsilon_i - \frac{1}{n} \sum_{j=1}^n \epsilon_j$  is the centered spectrum  $(\sum_{i=1}^n \tilde{\epsilon}_i = 0)$ . Equation (B6) holds insofar  $f_i^2 \ge 0 \forall i$ , i.e.,

$$J \geqslant J_n^c = n\tilde{\epsilon_n},\tag{B7}$$

where  $n\tilde{\epsilon}_n = \sum_{j=1}^{n-1} \epsilon_n - \epsilon_j$  is the sum of energy differences with all lower levels. Repeating the procedure for a solution with just the first *m* levels occupied, the same expressions (B6)–(B7) are obtained with  $n \to m$ .

# APPENDIX C: SPLITTING OF ENERGY LEVELS AT THE BORDER OF FACTORIZATION

Let us assume that  $H = H_f + \delta H$ , where  $H_f = H_0 + V_{int}$  is the Hamiltonian having the factorized GS and

$$\delta H_0 = \sum_i \delta \epsilon_i \sum_p c^{\dagger}_{pi} c_{pi}, \qquad (C1)$$

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a small perturbation of the single-particle term. For instance, a perturbation  $\delta V_{\text{int}} = \gamma V_{\text{int}}$  leads to  $\delta H = \gamma H_f - \gamma H_0$ , implying  $\delta \epsilon_i = -\gamma \epsilon_i$  plus a constant energy shift  $\delta E = \gamma E_f$ .

At first order in  $\delta \epsilon_i$ , the remaining correction on the definite parity energy levels is

$$\delta E_{\sigma_2,\dots,\sigma_n} = \sum_i \delta \epsilon_i \langle N_i \rangle_{\sigma_2,\dots,\sigma_n}, \tag{C2}$$

° N 1-

where  $N_i = \sum_p c_{pi}^{\dagger} c_{pi}$  and the average is taken on the parity projected states (57). For n = 3,  $\langle N_i \rangle_{\sigma_2,\sigma_3} / N$  is given in Eq. (62). We then obtain, setting  $u_i = 1 - 2|f_i|^2$ ,

$$\frac{\delta E_{\sigma_2 \sigma_3}}{N} = \frac{\sum_i \delta \epsilon_i |f_i|^2 \left[1 + \sum_j \sigma_j (-1)^{\delta_{ji}} u_j^{N-1}\right]}{1 + \sum_j \sigma_j u_j^N}$$
$$\approx \sum_i \delta \epsilon_i |f_i|^2 \left[1 + \sum_j \sigma_j \left[(-1)^{\delta_{ji}} + 2|f_j^2| - 1\right] u_j^{N-1}\right],$$

where  $\sigma_1 \sigma_2 \sigma_3 = (-1)^N$  and the last expression holds for sufficiently large *N*. For  $\delta \epsilon_3 = -\delta \epsilon_1 = \delta \epsilon$  and  $\delta \epsilon_2 = 0$ , this leads to  $\delta E_{++} < \delta E_{-+} < \delta E_{+-}$  for  $\delta \epsilon > 0$ . This is the case of Fig. 2, where  $\delta \epsilon = (1 - \frac{v}{v_c})\epsilon > 0$  (<0) on the left (right) side of the factorization point  $v = v_c$ . In the V = 0 case,  $\langle N_i \rangle = n_i$  is just the occupation of level *i* in the projected states (51) and (52), and (C2) becomes exact.

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