Gauge-Canonical PEPS Ansatz for a Square-Lattice Rydberg Blockade Model

Bipartite (A/B) and Directed (L,U in; R,D out) Formulations

(technical note)

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Abstract

We document two PEPS parameterizations for a hard Rydberg blockade model on the square lattice (nearest-neighbor exclusion): (i) a bipartite *A/B* formulation and (ii) a directed-edge formulation with *incoming* virtual legs (L, U) and *outgoing* legs (R, D). Both are "gauge-canonical" in the sense that the blockade constraint is enforced by fixed, parameter-free Kronecker-δ / filter structures, so that forbidden configurations have exactly zero amplitude for *all* variational parameters. The directed formulation is illustrated with explicit figures. A short appendix explains the relation to the gauge canonical form (GCF) used for Abelian lattice gauge theory PEPS in Wu–Liu (2025).

1 Model and constraint

Consider a square lattice with a two-level Rydberg degree of freedom at each site i, with computational basis $|n_i\rangle$, $n_i \in \{0, 1\}$. The hard blockade constraint forbids simultaneous excitations on nearest neighbors:

$$n_i n_j = 0 \quad \text{for every nearest-neighbor edge } \langle ij \rangle. \tag{1}$$

Equivalently, the physical Hilbert space is the *independent-set* subspace

$$\mathcal{H}_{\mathrm{IS}} = \mathrm{span}\{|s\rangle : \ s = \{n_i\} \in \mathcal{I}\}, \qquad \mathcal{I} = \{s : \ n_i n_j = 0 \ \forall \langle ij \rangle\}. \tag{2}$$

In variational Monte Carlo (VMC) one typically samples only $s \in \mathcal{I}$, and thus never needs to evaluate wavefunction amplitudes on forbidden configurations. Nevertheless, it is advantageous to build an ansatz whose amplitude *vanishes exactly* for $s \notin \mathcal{I}$ at the parameterization level; this removes redundant degrees of freedom associated with "nonphysical" amplitudes.

2 PEPS notation and virtual-sector decomposition

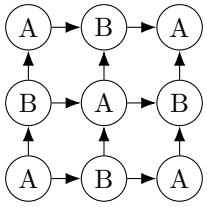
A (finite) PEPS defines amplitudes

$$\Psi(s) = \langle s|\Psi|s|\Psi\rangle = \mathrm{tTr}\Big[\prod_i T^{[i]}_{n_i} \Big], \tag{3}$$

where $T^{[i]}_{n_i}$ is the local tensor at site i with its physical index fixed to n_i, and tTr denotes contraction of all virtual bonds.

To encode the blockade constraint in a gauge-canonical way, we decompose each virtual bond space into two *sectors* $k \in \{0, 1\}$ (interpreted as "neighbor not excited" / "neighbor excited") with a possible degeneracy in each sector. Concretely, each virtual index is taken as

$$a \equiv (k, \mu), \qquad k \in \{0, 1\}, \qquad \mu = 1, \ldots, D_k, \tag{4}$$



Bipartite lattice (schematic).
Each bond connects A to B.

Figure 1: Schematic A/B bipartition used in the bipartite formulation. The arrows are only illustrative (one may treat the bonds as undirected); the essential ingredient is that every bond connects an A site to a B site.

so the total bond dimension is $D = D_0 + D_1$. The numbers D_k are the *degeneracies* (or sector dimensions). The key point is that the blockade logic uses only the sector label k, while the degeneracy indices μ carry the variational "entanglement capacity".

We further define a fixed *filter* function

$$v_k(n) = \begin{cases} 1, & k = 0, \\ 1 - n, & k = 1, \end{cases} \qquad n \in \{0, 1\}. \tag{5}$$

Thus, if a site is proposed to be excited ($n = 1$) while it receives a sector-1 message ($k = 1$), then $v_1(1) = 0$ kills the amplitude.

3 Bipartite formulation (A/B)

3.1 Lattice bipartition and philosophy

On a bipartite square lattice, label sublattices as A and B so that every nearest-neighbor bond connects an A site to a B site. The A/B formulation implements the blockade as a *copy–filter* mechanism:

- On an A site, the tensor *copies* its occupation n into the sector label k on all adjacent bonds.
- On a B site, the tensor *filters*: if it is excited ($n = 1$), it requires that all neighbor sectors are $k = 0$.

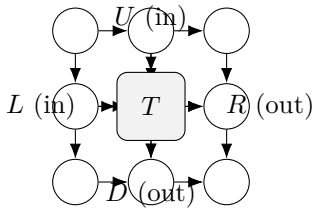
The resulting ansatz has exactly zero amplitude whenever an adjacent pair of excitations appears.

3.2 A-sublattice tensor: copy to sectors

Let the four virtual legs be labeled (L, R, U, D) and each index be $a_e = (k_e, \mu_e)$. On an A site we define

$$T^{[A]}_{n;\,(k_L,\mu_L)(k_R,\mu_R)(k_U,\mu_U)(k_D,\mu_D)} = \Big[\prod_{e\in\{L,R,U,D\}} \delta_{k_e,n} \Big] \, A^{[A]}_{n;\,\mu_L\mu_R\mu_U\mu_D}, \tag{6}$$

where the core tensors $A^{[A]}_n$ are variational parameters. Equation (**??**) enforces that all adjacent bond sectors equal the physical occupation n on A.



Directed convention: L, U incoming; R, D outgoing.

Figure 2: Directed-edge convention for the translation-invariant formulation: all horizontal bonds are oriented left→right and all vertical bonds top→bottom. For the highlighted tensor T, legs (L, U) are incoming and (R, D) are outgoing.

3.3 B-sublattice tensor: filter

On a B site we impose a filtering structure. A convenient (general) canonical choice is

$$T^{[B]}_{n;\,(k_L,\mu_L)(k_R,\mu_R)(k_U,\mu_U)(k_D,\mu_D)} = \Big[\prod_{e\in\{L,R,U,D\}} v_{k_e}(n)\Big]\; B^{[B]}_{n;\,k_L k_R k_U k_D;\,\mu_L\mu_R\mu_U\mu_D}. \tag{7}$$

Because $v_1(1) = 0$, if the B site is excited ($n = 1$), then every adjacent sector must satisfy $k_e = 0$. The tensor blocks $B^{[B]}_{n;\,k_L k_R k_U k_D}$ are the variational parameters, but they are only sampled in the sector combinations compatible with the physical configuration.

3.4 Exact blockade

Consider a nearest-neighbor bond connecting an A site i to a B site j. From the A tensor, the shared sector on that bond is fixed to $k = n_i$ by the δ constraint. If both sites were excited ($n_i = n_j = 1$), then the B tensor contributes a factor $v_k(n_j) = v_1(1) = 0$, hence $\Psi(s) = 0$. Therefore the amplitude vanishes identically for any configuration containing an adjacent pair of excitations.

4 Directed formulation: (L, U) incoming, (R, D) outgoing

4.1 Directed-edge convention

Fix a *global* orientation of the square lattice bonds so that at every site:

- the **incoming** virtual legs are *Left* (L) and *Up* (U);
- the **outgoing** virtual legs are *Right* (R) and *Down* (D).

Equivalently, every horizontal bond is oriented left→right, and every vertical bond is oriented top→bottom. This choice makes every site both a receiver (from L, U) and a sender (to R, D), while keeping a single, translation-invariant tensor type.

4.2 Local tensor definition (gauge-canonical form)

Each virtual leg carries an index $a = (k, \mu)$ with $k \in \{0, 1\}$ and $\mu = 1, \ldots, D_k$. Define a single site tensor (valid for all sites) as

$$\begin{aligned} &T_{n;\,(k_L,\mu_L)(k_U,\mu_U)(k_R,\mu_R)(k_D,\mu_D)} \\ &\quad= \underbrace{\delta_{k_R,n}\,\delta_{k_D,n}}_{\text{copy to outgoing sectors}}\;\underbrace{v_{k_L}(n)\,v_{k_U}(n)}_{\text{filter incoming sectors}}\;\times C^{(k_L,k_U)}_{n;\,\mu_L\mu_U\mu_R\mu_D}. \end{aligned} \tag{8}$$

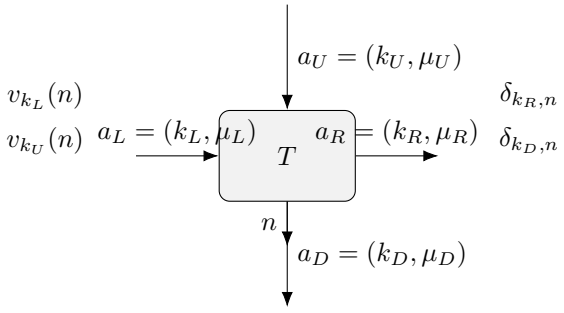


Figure 3: Structure of the directed-formulation site tensor (**??**). Outgoing sectors (R, D) are fixed to the physical occupation by Kronecker deltas, while incoming sectors (L, U) are filtered by $v_k(n)$ with $v_1(1) = 0$. The degeneracy indices μ carry the variational core tensor $C_n^{(k_L,k_U)}$.

Here $C_n^{(k_L,k_U)}$ is the variational *core tensor* (degeneracy part), while all δ and v_k factors are fixed and parameter-free.

4.3 Block structure

Equation (**??**) implies a sparse block structure:

- If $n = 1$, the filter factors enforce $k_L = k_U = 0$ (since $v_1(1) = 0$), while the deltas enforce $k_R = k_D = 1$. Thus there is a *single* nonzero sector pattern:

$$(n = 1): \quad (k_L, k_U, k_R, k_D) = (0, 0, 1, 1), \tag{9}$$

  with core block shape $D_0 \times D_0 \times D_1 \times D_1$ (for $\mu_L, \mu_U, \mu_R, \mu_D$).

- If $n = 0$, the deltas enforce $(k_R, k_D) = (0, 0)$, while $(k_L, k_U) \in \{0, 1\}^2$ are allowed. So there are four $n = 0$ blocks labelled by (k_L, k_U), with shapes $D_{k_L} \times D_{k_U} \times D_0 \times D_0$.

The key algorithmic property is that, for any fixed physical configuration s, the sector labels k on every bond are uniquely fixed by the source site (because of the outgoing deltas). Hence the single-layer network $\langle s|\Psi|s|\Psi\rangle$ contracts only the corresponding degeneracy dimensions.

4.4 Exact blockade: local two-site argument

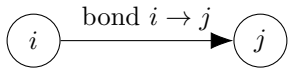
Consider a directed bond $i \to j$ (either horizontal or vertical). By the outgoing constraints at i, the bond sector equals the occupation:

$$k_{i\to j} = n_i. \tag{10}$$

At site j this sector enters as an incoming leg (either L or U), contributing a factor $v_{k_{i\to j}}(n_j)$. If both sites are excited ($n_i = n_j = 1$), then $k_{i\to j} = 1$ and

$$v_{k_{i\to j}}(n_j) = v_1(1) = 0, \tag{11}$$

so the amplitude vanishes. Therefore $\Psi(s) = 0$ for any configuration containing an adjacent 11, independently of the variational core tensor C.



$$n_i = 1 \Rightarrow k_{i\to j} = 1 \text{ (outgoing } \delta\text{)}$$

$$n_j = 1 \Rightarrow v_{k_{i\to j}}(n_j) = v_1(1) = 0 \text{ (incoming filter)}$$

Figure 4: Two-site mechanism enforcing the blockade in the directed formulation. If i is excited, the outgoing delta fixes the bond sector to $k = 1$. If j is also excited, the incoming filter produces $v_1(1) = 0$, killing the amplitude.

5 Remarks on redundancy and SR stability

The constructions above remove redundancy associated with amplitudes of forbidden configurations: those amplitudes are identically zero at the ansatz level, so there are no parameters whose only role would be to tune nonphysical weights.

A separate and unavoidable issue is the intrinsic *PEPS gauge redundancy* on internal virtual bonds: inserting X and X^{-1} on a bond leaves the physical state invariant. In stochastic reconfiguration (SR) or time-dependent VMC (tVMC), the infinitesimal generators of these gauge transformations appear as null vectors of the log-derivative matrix and the quantum geometric tensor. Analytic gauge removal procedures (e.g. QR projection or minSR formulations) can be used to stabilize the SR equation.

A Relation to the gauge canonical form for lattice gauge theory PEPS (minimal)

Wu and Liu (2025) formulate gauge-invariant PEPS for Abelian lattice gauge theories by assigning a conserved *charge* to each virtual index and enforcing a local Gauss-law constraint as a block-sparsity condition. In their notation, the bond dimension decomposes as

$$D = \sum_k D_k, \tag{12}$$

where D_k is the *degeneracy* (multiplicity) of charge sector k (the number of virtual basis states carrying charge k). They further identify a *gauge canonical form* (GCF) in which the link (gauge) tensor becomes parameter-free:

$$B^n_{lr} = \delta_{lr}\, \delta_{n,q(l)}\, \delta_{n,q(r)}, \tag{13}$$

so only the matter tensors remain variational. In VMC, each sampled physical configuration uniquely selects the charge sector on each bond; consequently, the effective bond dimension of the single-layer network reduces from the total D to the relevant D_k on that bond, providing a substantial computational simplification.

The Rydberg-blockade PEPS constructions above are a direct analogue of this logic. The sector label $k \in \{0, 1\}$ plays the role of the "charge" (or electric-field value) carried by a virtual index. The fixed delta / filter structures in Eqs. (**??**)–(**??**) are the blockade counterpart of the parameter-free GCF link tensor: they enforce the hard constraint and remove variational parameters from the constraint part of the ansatz. The remaining degeneracy indices μ correspond to the degeneracy dimensions D_k in the gauge-theory setting. Finally, because outgoing deltas (or the bipartite copy tensor) fix sector values bond-by-bond, every sampled independent-set configuration selects a unique sector pattern, so that the single-layer contraction only involves

the corresponding D_k channels, exactly mirroring the "configuration selects sector" feature emphasized in the lattice gauge theory PEPS literature.

Reference. Y. Wu and W.-Y. Liu, *Accurate Gauge-Invariant Tensor-Network Simulations for Abelian Lattice Gauge Theory in (2+1)D: Ground-State and Real-Time Dynamics*, Phys. Rev. Lett. **135**, 130401 (2025).