Smart Sampling of Independent Sets in Rydberg-Blockaded Atom Arrays in Variational Monte Carlo Summary January 6, 2026

One-line goal. Aim to sample independent sets $n \in \mathcal{I}(G)$ from the Born distribution $\pi_{\theta(n)} \propto \left|\psi_{\theta(n)}\right|^2$ to obtain lower-variance, lower-autocorrelation estimators in VMC for Rydberg blockade Hamiltonians.

1. Background: Rydberg blockade as an independent-set constraint

In the strong blockade regime, a Rydberg array with binary occupation variables $n_i \in \{0,1\}$ admits only configurations in which no two excited atoms violate the blockade radius. Defining a graph $G = (V, E)$ where $(i,j) \in E$ when atoms i, j are within the blockade distance, the allowed configurations coincide with independent sets:

$$\mathcal{I}(G) = \left\{n \in \{0,1\}^{\{|V|\}} : n_i n_j = 0 \forall (i,j) \in E\right\}.$$

This is a common mapping used to encode (maximum) independent set optimization on Rydberg hardware.

VMC optimization of a variational state $\psi_{\theta(n)}$ requires samples from

$$\pi_{\theta(n)} = \frac{\left|\psi_{\theta(n)}\right|^2}{Z_\theta}, \quad n \in \mathcal{I}(G), \quad Z_\theta = \sum_{n \in \mathcal{I}(G)} \left|\psi_{\theta(n)}\right|^2.$$

The primary practical issue is constructing samplers that (i) respect the hard constraint, (ii) mix across near-degenerate patterns (e.g., ordered/stripe phases), and (iii) remain computationally practical given the expense of evaluating ψ_θ.

2. Why sampling is hard in practice

Independent-set spaces become rugged when the target distribution is strongly biased toward high-density configurations or when multiple symmetry-related patterns compete. Common failure modes include:

- **Low acceptance at high density:** most empty vertices are blocked, so insertions are rarely valid.
- **Collective slow modes:** changing between stripe or checkerboard-like patterns requires moving many excitations coherently; single-site flips diffuse.
- **Multimodality:** distinct basins separated by entropic barriers lead to metastability and long autocorrelation times.

3. Smart methods: a practical catalogue

3.1. A. Local, constraint-aware updates (baseline, inexpensive)

A1. Insert-delete Metropolis (Glauber-like) with fast constraint checks. Maintain (i) adjacency lists $\mathcal{N}(i)$ and (ii) a blocked count $b_i = \sum_{j \in \mathcal{N}(i)} n_j$. Then insertion at i is allowed iff $b_i = 0$.

For a proposal $n \to n'$, accept with

$$\alpha = \min\left(1, \frac{\left|\psi_{\theta(n')}\right|^2}{\left|\psi_{\theta(n)}\right|^2} \cdot \frac{q(n \mid n')}{q(n' \mid n)}\right).$$

A2. Single-site heat-bath (Gibbs) updates (often better). At a chosen site i, consider the two configurations differing only in n_i. If $b_i > 0$, the $n_i = 1$ option has zero weight. Otherwise, sample

$$\Pr(n_i = 1 \mid n_{-i}) = \frac{\left|\psi_{\theta(n^1)}\right|^2}{\left|\psi_{\theta(n^0)}\right|^2 + \left|\psi_{\theta(n^1)}\right|^2}.$$

This is rejection-free and can reduce wasted evaluations when Metropolis acceptance is low.

A3. Locally balanced / informed site selection. Bias the choice of update site toward flippable locations or those with large expected amplitude ratio. Correct any asymmetry with the proposal ratio. This is a relatively low-engineering way to raise acceptance.

3.2. B. Swap / pivot moves (high impact near maximal independent sets)

When insertions are rare, add moves that keep density approximately fixed:

- Pick an empty vertex v blocked by exactly one occupied neighbor u.
- Propose a swap $n' = n - \{u\} + \{v\}$.

This can allow efficient surface diffusion along near-maximal independent sets and is often helpful in MIS-like regimes.

3.3. C. Patch / strip (block) updates to destroy domain walls

To accelerate collective rearrangements, propose updates that rewrite an entire region $P \subset V$ while keeping the boundary fixed.

Patch proposal template.

1. Choose a patch P (e.g., a kxk square in a 2D array or a stripe).
2. Remove occupations inside P, keep ∂P fixed.
3. Propose a new independent-set pattern in P given the boundary using a fast proposal q_P:
   - dynamic programming / transfer-matrix for narrow stripes,
   - precomputed enumeration for very small patches.
4. Accept with MH using the global $|\psi_\theta|^2$ ratio and q_P ratio.

Inspiration from classical hard-core gases. Rejection-free strip updates that evaporate all particles in a strip and reoccupy it efficiently sample low-entropy/high-density regimes in hard-core lattice gases; the same move geometry is often useful as a proposal inside VMC.

3.4. D. Rejection-free kinetic scheduling (n-fold way / BKL)

When invalid or rejected proposals dominate, use rejection-free event selection. Define a set of allowed move types m with rates $r_{m(n)}$ that satisfy (global or detailed) balance with respect to π_θ. Sample the next move according to rates and update the configuration without rejection. This can improve efficiency when acceptance is small.

3.5. E. Tempering / population strategies for multimodality

Parallel tempering in a Born exponent. Run replicas targeting

$$\pi_{\theta,\beta}(n) \propto \left|\psi_{\theta(n)}\right|^{2\beta}, \quad 0 < \beta \leq 1.$$

and occasionally swap neighboring β-replicas with replica-exchange acceptance. Smaller β flattens the landscape and helps the chain traverse between modes.

3.6. F. Learned global proposals (flows or other generative models) with MH correction

When the wavefunction is not directly sampleable, train a separate proposal model $q_{\varphi(n)}$ over $\mathcal{I}(G)$ (e.g., a flow-based generator). Use independence Metropolis-Hastings:

$$\alpha = \min\left(1, \frac{\left|\psi_{\theta(n')}\right|^2 q_{\varphi(n)}}{\left|\psi_{\theta(n)}\right|^2 q_{\varphi(n')}}\right).$$

Mixing local kernels with occasional global proposals can reduce autocorrelation when $|\psi_\theta|^2$ is multi-modal.

4. A recommended sampler "stack" for Rydberg-VMC

A practical starting point is a mixture kernel combining complementary moves:

- **Every sweep:** single-site Gibbs (or insert-delete MH) using flippable-site lists.
- **Every few sweeps:** swap/pivot moves to improve mobility at high density.
- **Periodically:** patch or stripe proposals (MH-corrected) to heal domain walls.
- **If bimodal or hysteretic:** parallel tempering in β on $|\psi|^{2\beta}$.
- **Optional:** learned global proposals (flows or other generative models) mixed into the kernel.

Rule of thumb. A move is often worthwhile if it reduces variance per unit cost. A patch move that is 10-20x more expensive than a local move can still be a net win if it reduces integrated autocorrelation times by 100x.

5. Implementation notes (engineering details that matter)

Data structures. For a geometric blockade graph (unit-disk-like), store adjacency lists and maintain blocked counts b_i. Maintain dynamic sets:

- occupied sites $\{i : n_i = 1\}$,
- insertable sites $\{i : n_i = 0, b_i = 0\}$,
- swappable pairs $(u \to v)$ where u is occupied, v is empty, and v is blocked by exactly one neighbor u.

These can be updated in $O(\deg(i))$ per accepted local move.

Amplitude ratios. Most MH or Gibbs decisions only require $\log(|\psi(n')|) - \log(|\psi(n)|)$. For local moves, consider caching or incremental evaluation whenever the ansatz supports it.

Diagnostics. Track integrated autocorrelation times τ_{int} for key observables (excitation number, structure factors, energy), and report effective sample size (ESS) per wall-clock second. Tune mixture weights to maximize ESS/sec.

6. Key references (entry points)

References

1. H. Pichler, S.-T. Wang, L. Zhou, S. Choi, and M. D. Lukin, "Quantum optimization for maximum independent set using Rydberg atom arrays," arXiv:1808.10816 (2018).
2. S. Ebadi et al., "Quantum optimization of maximum independent set using Rydberg atom arrays," Science 376, 1209-1215 (2022).
3. A. B. Bortz, M. H. Kalos, and J. L. Lebowitz, "A new algorithm for Monte Carlo simulation of Ising spin systems," J. Comput. Phys. 17, 10-18 (1975).

4. M. S. Albergo, G. Kanwar, and P. E. Shanahan, "Flow-based generative models for Markov chain Monte Carlo in lattice field theory," Phys. Rev. D 100, 034515 (2019).
5. A. A. A. Jaleel, J. E. Thomas, D. Mandal, Sumedha, and R. Rajesh, "Rejection-free cluster Wang-Landau algorithm for hard-core lattice gases," Phys. Rev. E 104, 045310 (2021).
6. M. Huber, "Spatial birth-death swap chains," Bernoulli 18(3), 1031-1041 (2012); arXiv:1006.5934.