Quantum Metropolis methods and thermalisation

Understand Metropolis-style thermal sampling and why the full quantum channel needs a correctness proof.

Research 21 min lesson Dr. Charith Jayasekara

By the end, you'll be able to

- Verify detailed balance in a two-state example.
- Explain why quantum rejection is not a classical undo.
- Distinguish historical proposals from corrected channel analyses.

Begin with the classical accept–reject idea

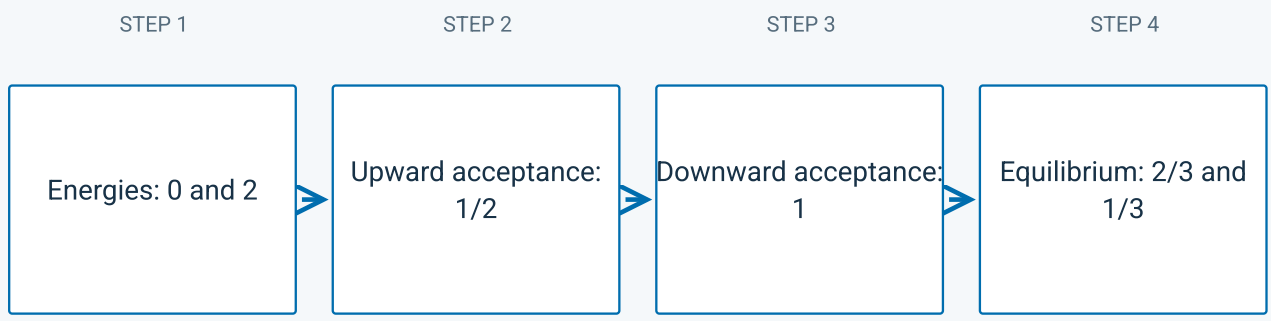
Classical Metropolis sampling explores configurations by proposing a move and accepting it according to an energy-dependent probability. Moves to lower energy are accepted, while some moves to higher energy are accepted so the process can explore rather than get stuck immediately. Under suitable proposal and convergence conditions, its stationary distribution has thermal Gibbs weights.

A quantum Hamiltonian complicates this story because energy eigenstates need not be ordinary configuration labels. Measuring energy can disturb superpositions, and rejecting a proposed move is not simply equivalent to restoring an erased classical variable. Quantum Metropolis proposals therefore need coherent energy estimation, carefully designed acceptance operations and a valid treatment of rejection.

Review measurement disturbance, reversibility and phase kickback. The goal is a thermal ensemble or thermal-state approximation, not a single deterministic minimum-energy answer.

WORKED DIAGRAM · AA14

Balanced thermal probability flow



At equilibrium, upward flow is (2/3)(1/2)=1/3 and downward flow is (1/3)(1)=1/3. Quantum implementations additionally need valid finite-precision energy and rejection operations.

State the thermal-sampling setup

Specify an implementable Hamiltonian, inverse temperature, proposal operations, energy-resolution requirement and final state error. State whether the algorithm outputs energy-eigenstate samples, a mixed state or estimates of thermal observables. A correctness proof needs both the intended equilibrium distribution and a convergence analysis under explicit assumptions.

Energy precision matters. An acceptance probability depends on an energy difference, so finite-resolution estimates change the implemented transition rule. Near-degenerate energies may be difficult to distinguish, and overly informative measurements can alter the state. A mathematically clean acceptance formula is only one component of a valid quantum channel.

Work a two-state classical analogue

Take energies zero and two, with symmetric proposals that always suggest switching states. Choose beta equal to natural logarithm of two divided by two. Moving downward is accepted with probability one. Moving upward is accepted with probability one half. The transition from ground to excited therefore has probability one half, while the reverse transition has probability one.

At equilibrium, the probability flow from ground to excited must equal the reverse flow. If the ground probability is two thirds and excited probability one third, the two flows are both one third. This is detailed balance for the example. It explains the Gibbs ratio without requiring any quantum circuit.

Now imagine the energies refer to unknown quantum eigenstates rather than stored classical labels. A proposal unitary can create a superposition of different energies. Estimating and accepting those components requires a coherent construction. If rejection has already disturbed the original state, simply applying the inverse proposal may not restore it. That is the key difficulty the quantum version must address.

For symmetric proposals, the classical acceptance rule makes upward and downward probability flows balance.

$$A(E \to E') = \min\{1, e^{-\beta(E'-E)}\}, \qquad \pi_0 A(0 \to 2) = \frac{2}{3} \cdot \frac{1}{2} = \frac{1}{3} = \frac{1}{3} \cdot 1 = \pi_2 A(2 \to 0).$$

Here $\beta = (\ln 2)/2$, and π_0, π_2 are the thermal equilibrium probabilities. This is a classical two-state check with symmetric proposals; the quantum channel still requires its own treatment of energy precision and rejection.

Historical proposal and a necessary correction

Temme and colleagues introduced an influential quantum Metropolis proposal using energy estimation and a quantum treatment of rejected moves. It is a foundational route toward thermal sampling, but its original correctness analysis should not be presented as an unconditional general theorem. Read the original proposal.

Jiang and Irani's *Quantum Metropolis Sampling via Weak Measurement*, accepted by PRX Quantum on 2 November 2026, identifies a problem with the earlier analysis's boosted, shift-invariant phase-estimation assumption and develops a weak-measurement approach with a different correctness argument. This distinction is essential when teaching the subject as of November 2026. Read the accepted primary paper.

The lesson is not that thermal sampling is impossible. It is that an attractive accept–reject analogy needs a complete quantum-channel proof, including finite energy precision and rejection behaviour. Research proposals, corrected constructions and implemented experiments are different kinds of evidence.

Follow a careful design review

First identify the target Gibbs state and observable. Specify the proposal family and show why it can connect the relevant energy sectors. Analyse the actual finite-precision channel, rather than an idealised acceptance rule alone. Establish its approximate fixed point, bound the error relative to the intended Gibbs state and study convergence. Finally account for the cost of each energy-estimation or weak-measurement step.

Detailed balance is a useful sufficient principle in many classical settings, but quantum constructions require the appropriate operator-level analysis. A correct stationary state also does not guarantee rapid mixing. The proposal may explore the state space slowly, especially across bottlenecks. Report any unproved mixing assumption separately from the state-correctness guarantee.

Know what a small demonstration establishes

A two-level experiment can show how energy-dependent acceptance behaves under controlled conditions. It cannot by itself establish scalability, rapid mixing or an advantage on difficult many-body systems. Compare against exact diagonalisation or classical sampling for the same small instance, then state which property the demonstration was intended to validate.

The phrase “avoids a sign problem” should also be used carefully. Removing one obstacle in a particular simulation representation does not prove a universally efficient algorithm for all thermal quantum systems. Other costs, including state preparation, spectral resolution and convergence, remain. A useful account identifies the obstacle being addressed and the assumptions that remain.

Keep proposal probabilities in the balance equation

The worked acceptance rule assumes symmetric proposals: suggesting the reverse move is as likely as suggesting the forward move. If proposal probabilities differ, the classical Metropolis–Hastings correction includes their reverse-to-forward ratio. Ignoring that factor can change the stationary distribution even before any quantum complication appears. This is a useful small-model check: write both directed probability flows, including proposal and acceptance factors, and verify that the intended equilibrium weights balance them. A quantum generalisation must preserve the assumptions of its own channel proof rather than importing an acceptance formula outside its stated setting.

Practice with answers

Exercise 1. Verify the equilibrium flow balance for the two-state example.

> Check the worked answer
>
> Ground-to-excited flow is two thirds times one half, or one third. Excited-to-ground flow is one third times one, also one third. The ratio of state weights matches the Boltzmann factor one half.

Exercise 2. Why is a formal acceptance probability insufficient to prove a quantum sampler correct?

Check the worked answer

The full operation must define a valid quantum channel, account for disturbance and rejected proposals, control energy-estimation errors and converge to the intended state. A classical acceptance formula alone does not establish those properties.

Check your understanding

PAUSE & THINK

Does writing the correct classical acceptance formula prove a quantum sampler correct?

- [ ] Yes
- [ ] No; disturbance, rejection and finite-precision channel behaviour must be analysed
- [ ] Only when β is positive

Answer: No; disturbance, rejection and finite-precision channel behaviour must be analysed. A complete quantum operation needs a valid channel and a proof of its fixed point and convergence. The acceptance probability alone is insufficient.

Sources

- Read the original proposal
- Read the accepted primary paper