Quantum Phase Transitions via Imaginary-Time Path Integrals

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***Abstract*—The one-dimensional transverse-field Ising model provides a paradigmatic example of a continuous quantum phase transition driven by quantum fluctuations [1, 3]. In this work, the model is studied using the imaginary-time path integral formalism, which maps the quantum system onto an anisotropic two-dimensional classical Ising model through the Suzuki–Trotter decomposition [2]. Classical Monte Carlo simulations are performed on the resulting spacetime lattice to investigate the evolution of the system as the transverse-field strength is varied across the critical point. Worldline configurations are used to visualize quantum fluctuations, while magnetization, Binder cumulants, correlation functions, and kink densities are measured to characterize the transition. The simulations identify a critical region near the exact critical coupling $g = \Gamma/J = 1$, where ferromagnetic order is lost and correlations become enhanced. A central result is the direct observation of instanton proliferation in imaginary time: tunneling events are rare in the ordered phase, increase strongly near criticality, and dominate the disordered phase. These results demonstrate how the quantum phase transition can be understood through the emergence of instantons in the path-integral representation and illustrate the broader correspondence between quantum critical phenomena and classical statistical mechanics.**

I. Introduction

Phase transitions are among the most important phenomena in condensed matter physics because they describe qualitative changes in the macroscopic behavior of many-body systems. While conventional phase transitions are driven by thermal fluctuations at finite temperature, quantum phase transitions occur at zero temperature and are driven entirely by quantum fluctuations. These transitions arise when a non-thermal control parameter is varied, causing the ground state of a quantum system to change abruptly. Near a quantum critical point, fluctuations become correlated over increasingly large length scales, producing universal behavior that is largely independent of microscopic details [1, 4].

One of the most important models exhibiting a quantum phase transition is the one-dimensional transverse-field Ising model (TFIM). The model consists of spins interacting through a nearest-neighbor ferromagnetic coupling while simultaneously experiencing a transverse magnetic field. The interaction term favors alignment of neighboring spins and promotes long-range ferromagnetic order, whereas the transverse field induces quantum tunneling between spin states and tends to disorder the system. The competition between these two effects produces a continuous quantum phase transition at the critical ratio

$$\left(\frac{\Gamma}{J}\right)_c = 1,$$

where J is the Ising coupling strength and Γ is the transverse-field strength [3].

Although the TFIM is a quantum mechanical model, it can be reformulated using the imaginary-time path integral formalism. Through the Suzuki–Trotter decomposition, the one-dimensional quantum system can be mapped onto an anisotropic two-dimensional classical Ising model, where the additional dimension corresponds to imaginary time [2]. This quantum-to-classical correspondence provides both a powerful conceptual framework and a practical computational approach, allowing quantum critical behavior to be studied using classical Monte Carlo techniques.

In the worldline representation produced by this mapping, quantum tunneling events appear as spin flips along the imaginary-time direction. These events, often referred to as instantons or kinks, provide a direct visual manifestation of quantum fluctuations. Their density is expected to increase as the transverse field strengthens, ultimately destroying ferromagnetic order and driving the system through the quantum critical point.

The objective of this project is to investigate the quantum phase transition of the transverse-field Ising chain using the imaginary-time path integral formulation and Monte Carlo simulation of the resulting classical model. By measuring observables such as the magnetization, Binder cumulant, correlation length, and instanton density, we seek to characterize the transition and explore how the proliferation of instantons is related to the loss of long-range order. Particular emphasis is placed on visualizing worldline configurations across different regions of the phase diagram and interpreting the quantum phase transition from the perspective of imaginary-time dynamics.

II. Theoretical Background

A. Transverse-Field Ising Model

The one-dimensional transverse-field Ising model is described by the Hamiltonian

$$\hat{H} = -J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \Gamma \sum_i \hat{\sigma}_i^x,$$

where $J > 0$ is the ferromagnetic nearest-neighbor coupling and Γ is the transverse magnetic field. The operators $\hat{\sigma}^z$ and $\hat{\sigma}^x$ are Pauli matrices acting on each lattice site.

The two terms in the Hamiltonian favor competing behaviors. The interaction term tends to align neighboring spins along the z-direction, producing a ferromagnetically ordered ground state. In contrast, the transverse-field term does not commute with the interaction term and induces quantum

fluctuations that continuously mix spin-up and spin-down configurations.

In the limit $\Gamma/J \ll 1$, the interaction energy dominates and the system develops long-range ferromagnetic order characterized by a nonzero magnetization. In the opposite limit $\Gamma/J \gg 1$, the transverse field dominates and the system enters a quantum paramagnetic phase in which the magnetization vanishes. Pfeuty's exact solution of the one-dimensional TFIM shows that the quantum critical point separating these phases occurs at

$$\Gamma_c = J.$$

This exact result serves as the primary benchmark for the numerical simulations performed in this work [3].

B. Suzuki–Trotter Mapping and Quantum–Classical Correspondence

To study the TFIM using Monte Carlo methods, the quantum partition function

$$Z = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right)$$

is rewritten using the Suzuki–Trotter decomposition [2]. Splitting the Hamiltonian into commuting and non-commuting components,

$$\hat{H} = \hat{H}_z + \hat{H}_x,$$

the partition function may be expressed as

$$e^{-\beta \hat{H}} = \lim_{M\to\infty} \left(e^{-\Delta\tau \hat{H}_z} e^{-\Delta\tau \hat{H}_x}\right)^M,$$

where

$$\Delta\tau = \frac{\beta}{M}$$

is the imaginary-time discretization.

By inserting complete sets of σ^z basis states between successive Trotter factors, the partition function becomes a sum over spin configurations defined on a two-dimensional lattice with coordinates (i, τ), where i labels the physical lattice site and τ labels the discrete imaginary-time slice. The resulting spin trajectories are known as worldlines.

Carrying out the standard derivation yields the effective classical partition function

$$Z = \sum_{\{s_{i,\tau}\}} \exp\left[K_s \sum_{i,\tau} s_{i,\tau} s_{i+1,\tau} + K_\tau \sum_{i,\tau} s_{i,\tau} s_{i,\tau+1}\right],$$

which is precisely the partition function of an anisotropic two-dimensional classical Ising model [2]. The effective couplings are

$$K_s = J\Delta\tau,$$

and

$$K_\tau = \frac{1}{2} \ln \coth(\Gamma\Delta\tau).$$

This mapping establishes the central correspondence underlying the project:

$$\text{1D Quantum TFIM} \quad \Longleftrightarrow \quad \text{2D Classical Ising Model.}$$

As a result, the quantum phase transition of the original system can be studied through classical statistical mechanics simulations on the worldline lattice.

C. Worldlines and Instantons

The imaginary-time path integral formulation provides a direct physical interpretation of quantum fluctuations. After the Suzuki–Trotter decomposition, each spin is represented by a sequence of variables

$$s_{i,\tau} = \pm 1,$$

defined on discrete imaginary-time slices. For a fixed lattice site i, the sequence

$$s_{i,1}, s_{i,2}, \ldots, s_{i,M}$$

forms a trajectory through imaginary time known as a *worldline*. The collection of all worldlines defines a spacetime configuration on the effective two-dimensional lattice.

In the ordered phase, neighboring imaginary-time spins are strongly aligned, causing worldlines to remain nearly straight over long intervals. Such configurations correspond to spins that experience relatively little quantum tunneling. As the transverse field increases, spin-flip events along the imaginary-time direction become more frequent, producing discontinuities or kinks in the worldlines.

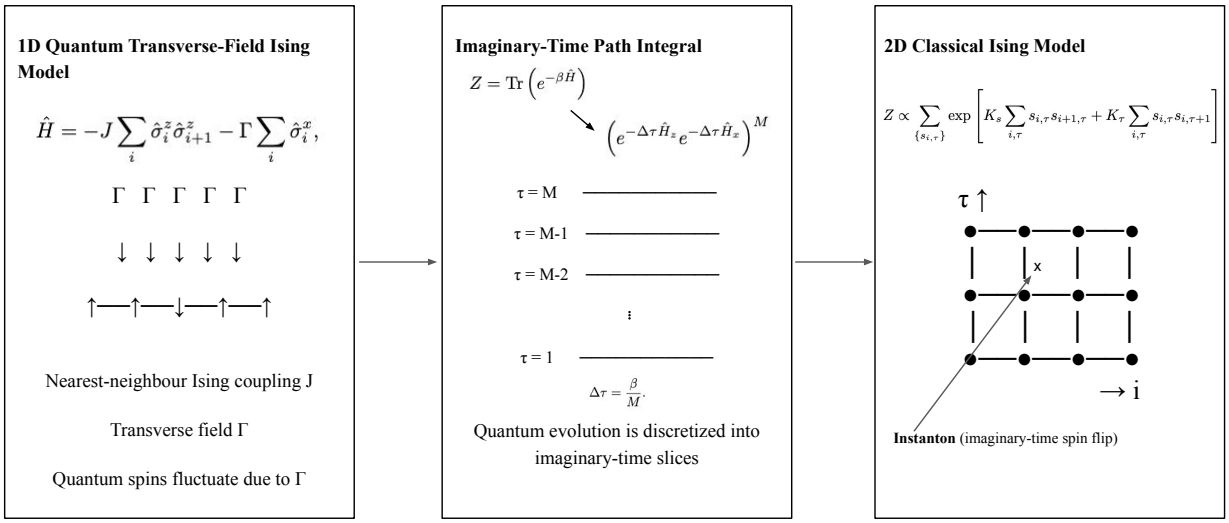
These kinks are commonly referred to as *instantons*. Within the path-integral picture, an instanton corresponds to a tunneling event between locally ordered spin configurations. Consequently, the density of instantons provides a direct measure of the strength of quantum fluctuations.

To quantify the abundance of these tunneling events, we define the kink density

$$n_{\mathrm{kink}} = \frac{1}{NM} \sum_{i,\tau} \frac{1 - s_{i,\tau} s_{i,\tau+1}}{2}.$$

This quantity counts the fraction of nearest-neighbor pairs along the imaginary-time direction that are anti-aligned. If a spin remains unchanged between adjacent time slices, the contribution is zero. If a spin flips, the contribution is unity. Therefore, n_{kink} directly measures the density of instantons present in a worldline configuration.

The worldline perspective provides an intuitive interpretation of the quantum phase transition. In the ferromagnetic phase, instantons are rare and worldlines remain largely coherent. Near the critical point, instantons proliferate and strongly disrupt long-range order. In the quantum paramagnetic phase, worldlines become highly fragmented, reflecting the dominance of quantum fluctuations. One of the central goals of this project is to investigate this instanton proliferation numerically and determine how it correlates with the disappearance of ferromagnetic order.



1D Quantum TFIM ↔ 2D Classical Ising Model

Fig. 1: Quantum-to-classical schematic mapping of the transverse-field Ising model. The one-dimensional quantum Hamiltonian is transformed via the Suzuki–Trotter decomposition into an anisotropic two-dimensional classical Ising model defined on a spacetime lattice (i, τ). Vertical worldlines represent imaginary-time spin histories, while kinks (instantons) correspond to quantum tunneling events. The resulting classical model exhibits the same critical point, $\Gamma_c/J = 1$, as the original quantum system.

III. Numerical Methodology

After mapping the transverse-field Ising model onto an anisotropic two-dimensional classical Ising model, the resulting partition function can be sampled using classical Monte Carlo techniques. The goal of the numerical simulations is to investigate how the effective spacetime configurations evolve as the dimensionless control parameter

$$g = \frac{\Gamma}{J}$$

is varied across the quantum critical point.

A. Simulation Lattice

The effective classical system is defined on a rectangular spacetime lattice with coordinates

$$(i, \tau),$$

where i labels the physical lattice site and τ labels the discrete imaginary-time slice. Each lattice variable satisfies

$$s_{i,\tau} = \pm 1.$$

Periodic boundary conditions were imposed in both the spatial and imaginary-time directions. The effective action is

$$S_{\text{eff}} = -K_s \sum_{i,\tau} s_{i,\tau}s_{i+1,\tau} - K_\tau \sum_{i,\tau} s_{i,\tau}s_{i,\tau+1},$$

with couplings

$$K_s = J\Delta\tau,$$

and

$$K_\tau = \frac{1}{2}\ln\coth(\Gamma\Delta\tau).$$

Throughout this work, the Trotter step was fixed at

$$\Delta\tau = 0.25,$$

and the imaginary-time extent was chosen to match the spatial system size,

$$M = L,$$

so that simulations remained approximately isotropic near the critical point.

B. Metropolis Monte Carlo Sampling

Configurations were generated using the Metropolis algorithm, a standard Markov-chain Monte Carlo method for sampling classical statistical systems [7]. Starting from an initial spin configuration, a lattice site (i, τ) was selected at random and a spin flip

$$s_{i,\tau} \to -s_{i,\tau}$$

was proposed.

The resulting change in the effective action,

$$\Delta S,$$

was computed from the nearest-neighbor interactions surrounding the selected site. The proposed move was then accepted with probability

$$P_{\mathrm{acc}} = \min\left(1, e^{-\Delta S}\right).$$

Repeated application of this procedure generates a Markov chain whose stationary distribution is proportional to the Boltzmann weight

$$e^{-S_{\mathrm{eff}}}.$$

For each value of g, an initial thermalization stage was performed before measurements were recorded. Observable averages were subsequently accumulated over many Monte Carlo sweeps separated by additional update cycles to reduce autocorrelation effects.

C. Measured Observables

Several observables were measured in order to characterize the quantum phase transition.

1) Magnetization: The order parameter was taken to be the average spin on the spacetime lattice,

$$m = \frac{1}{NM} \sum_{i,\tau} s_{i,\tau}.$$

Because finite systems may tunnel between positive and negative magnetization sectors, the quantity

$$|m|$$

was used when characterizing the ordered phase.

2) Energy: The energy density of the effective classical model was computed from the action per lattice site,

$$e = -\frac{1}{NM}\left[K_s \sum_{i,\tau} s_{i,\tau} s_{i+1,\tau} + K_\tau \sum_{i,\tau} s_{i,\tau} s_{i,\tau+1}\right].$$

Although this quantity is not identical to the quantum ground-state energy, it provides a useful diagnostic of changes in the effective classical ensemble.

3) Kink Density: To quantify instanton proliferation, the kink density was measured using

$$n_{\mathrm{kink}} = \frac{1}{NM} \sum_{i,\tau} \frac{1 - s_{i,\tau} s_{i,\tau+1}}{2}.$$

This observable counts spin flips along the imaginary-time direction and therefore directly measures the density of tunneling events.

4) Binder Cumulant: To locate the critical region, the fourth-order Binder cumulant was computed,

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}.$$

Binder cumulants for different system sizes are expected to intersect near the critical point, providing a finite-size estimate of

$$g_c.$$

This method is a standard finite-size diagnostic in Monte Carlo studies of phase transitions [7].

5) Correlation Functions: Spatial correlations were measured using the connected correlation function

$$C(r) = \langle s_i s_{i+r} \rangle - \langle s_i \rangle^2.$$

Away from criticality, correlations are expected to decay approximately exponentially,

$$C(r) \sim e^{-r/\xi},$$

allowing an estimate of the correlation length ξ to be extracted through numerical fitting.

D. Simulation Parameters

Simulations were performed over a range of transverse-field strengths spanning both the ordered and disordered phases. System sizes between

$$L = 16$$

and

$$L = 40$$

were used for finite-size comparisons, with corresponding imaginary-time extents

$$M = L.$$

The primary control parameter was

$$g = \Gamma / J,$$

which was varied across the expected critical value

$$g_c = 1.$$

The resulting data were used to construct worldline visualizations, magnetization curves, kink-density measurements, Binder-cumulant crossings, and correlation-length estimates.

IV. Results

A. Worldline Configurations Across the Phase Diagram

A major advantage of the imaginary-time path integral formulation is that it provides a direct visualization of quantum fluctuations through worldline configurations. Since each spin is represented by a trajectory in imaginary time, the resulting spacetime lattice offers an intuitive picture of how the system evolves as the transverse field is increased.

Figure 2 shows representative worldline configurations for three values of the control parameter,

$$g = \Gamma/J,$$

corresponding to the ordered phase, the critical region, and the disordered phase.

For

$$g = 0.3,$$

the system lies deep within the ferromagnetic phase. The worldlines remain nearly straight along the imaginary-time direction, indicating that tunneling events are rare. The configuration is dominated by large regions of uniform spin orientation, consistent with long-range ferromagnetic order. Quantitatively, the measured magnetization remains close to unity while the kink density is extremely small.

Near the critical point,

$$g = 1,$$

the structure of the worldlines changes dramatically. Extended domains begin to fragment and a substantial number of kinks appear along the imaginary-time direction. These instantons correspond to tunneling events between competing ordered configurations. The system exhibits strong fluctuations on many length scales, which is characteristic of critical behavior.

For

$$g = 2,$$

the transverse field dominates the dynamics and the system enters the quantum paramagnetic phase. The worldlines become highly fragmented, reflecting the proliferation of instantons throughout the spacetime lattice. Long-range ferromagnetic order is destroyed and the magnetization is strongly suppressed. The visual appearance of the configuration is qualitatively consistent with a disordered classical Ising system.

These worldline configurations provide direct evidence that increasing the transverse field enhances quantum tunneling. From the path-integral perspective, the quantum phase transition may therefore be viewed as a transition from a regime of rare instantons to one in which instantons proliferate and disrupt long-range order.

B. Magnetization and Instanton Proliferation

To quantify the evolution of the system across the quantum phase transition, we measured both the magnetization and the kink density as functions of the dimensionless control parameter

$$g = \Gamma/J.$$

The magnetization serves as the order parameter of the transition, while the kink density directly measures the abundance of instantons in the imaginary-time representation. Together, these observables provide complementary perspectives on the same physical phenomenon: the competition between ferromagnetic ordering and quantum tunneling.

Figure 3 shows the measured magnetization and kink density across the phase diagram.

For small values of g, the magnetization remains close to unity, indicating strong ferromagnetic order throughout the spacetime lattice. In this regime, the transverse field is weak and only a small number of instantons are present. The worldlines therefore remain largely coherent over long imaginary-time intervals.

As the transverse field approaches

$$g \approx 1,$$

the magnetization begins to decrease significantly. This reduction is accompanied by a rapid increase in the kink density, indicating that tunneling events become increasingly common. The onset of substantial instanton activity coincides with the destruction of long-range order, suggesting a direct connection between quantum fluctuations and the phase transition.

Beyond the critical region, the magnetization becomes strongly suppressed while the kink density continues to increase. In the disordered phase, the system is dominated by quantum fluctuations generated by the transverse field. The worldline configurations become highly fragmented and the ordered ferromagnetic state is no longer energetically favorable.

The simultaneous behavior of these observables provides strong support for the central physical interpretation of the project. From the perspective of the path-integral formulation, the quantum phase transition is not simply characterized by a vanishing order parameter. Rather, it may be understood as the proliferation of instantons in imaginary time. As the density of tunneling events increases, coherent ferromagnetic domains are progressively disrupted until long-range order is destroyed.

This interpretation is consistent with the worldline visualizations presented in Figure 2, where the transition from ordered to disordered behavior is accompanied by a dramatic increase in the number of imaginary-time spin flips.

C. Binder Cumulant Analysis

To further investigate the location of the critical region, Binder cumulants were computed for several system sizes. The Binder cumulant is defined as

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2},$$

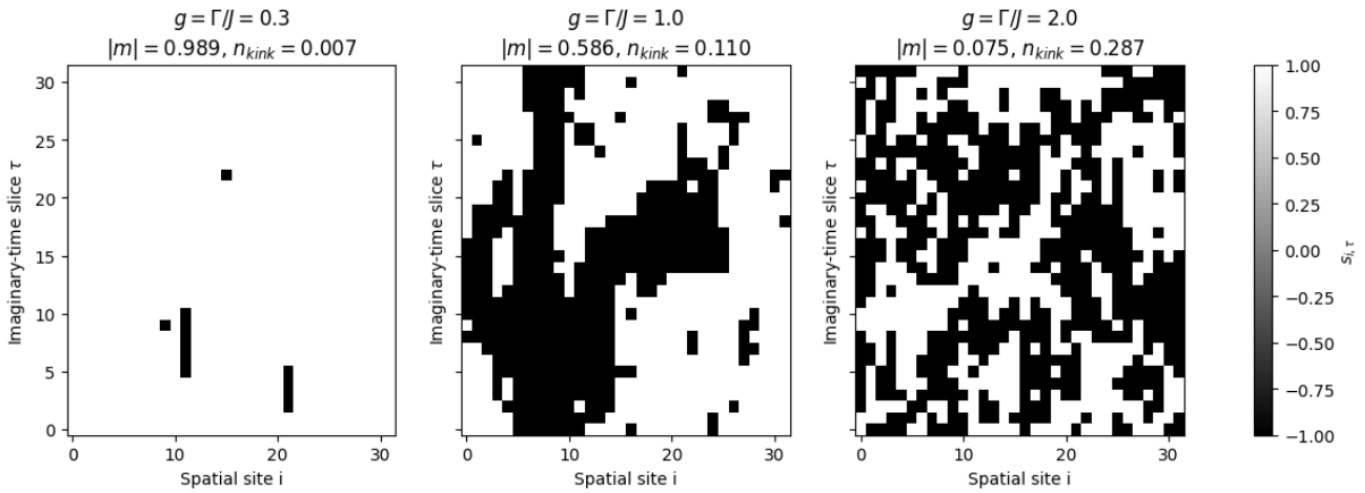


Fig. 2: Representative worldline configurations for the effective classical Ising model obtained from the imaginary-time path integral formulation of the transverse-field Ising chain. White and black regions correspond to opposite spin orientations. From left to right: ordered phase ($g = 0.3$), critical region ($g = 1.0$), and disordered phase ($g = 2.0$). The increasing fragmentation of worldlines reflects the growing density of instantons as the transverse field is increased.

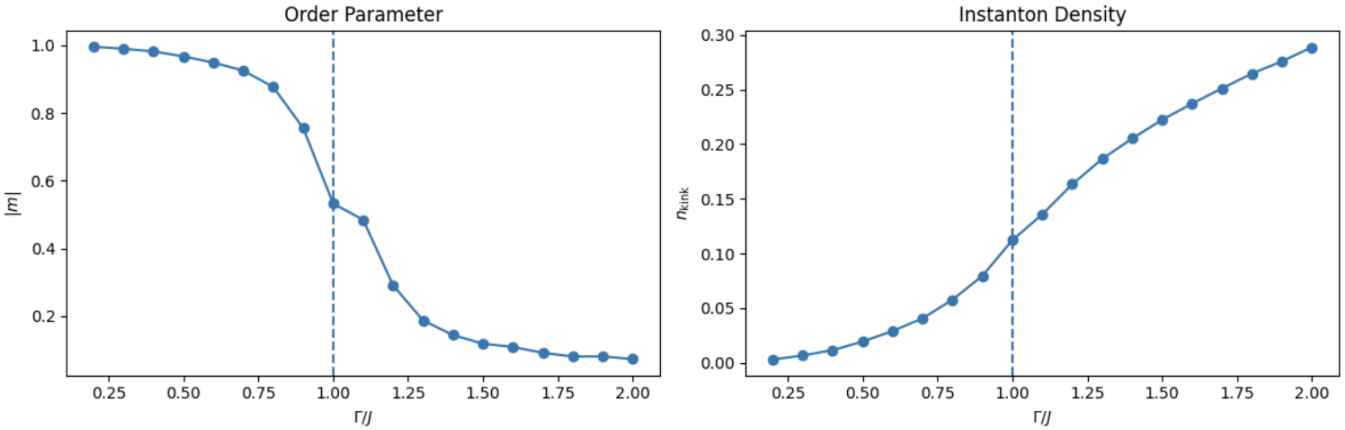


Fig. 3: Magnetization and kink density as functions of the transverse-field strength $g = \Gamma/J$. The vertical dashed line indicates the exact critical point $g_c = 1$. As the transverse field increases, the magnetization decreases while the density of instantons increases. The opposing behavior of these observables suggests that the loss of ferromagnetic order is driven by the proliferation of quantum tunneling events.

and provides a useful finite-size diagnostic for continuous phase transitions [7]. In the thermodynamic limit, Binder cumulants corresponding to different system sizes are expected to intersect at the critical point. Consequently, Binder crossings are frequently used to estimate critical couplings in Monte Carlo studies.

Figure 4 shows the Binder cumulant as a function of the transverse-field strength for system sizes ranging from

$$L = 16$$

to

$$L = 40.$$

For small values of g, all system sizes exhibit Binder cumulants close to

$$U_4 \approx \frac{2}{3},$$

which is characteristic of an ordered phase with a well-defined magnetization. As the transverse field increases, the Binder cumulant decreases and eventually approaches values associated with a disordered state.

The most important feature of Figure 4 is the clustering of the curves near

$$g \approx 1.$$

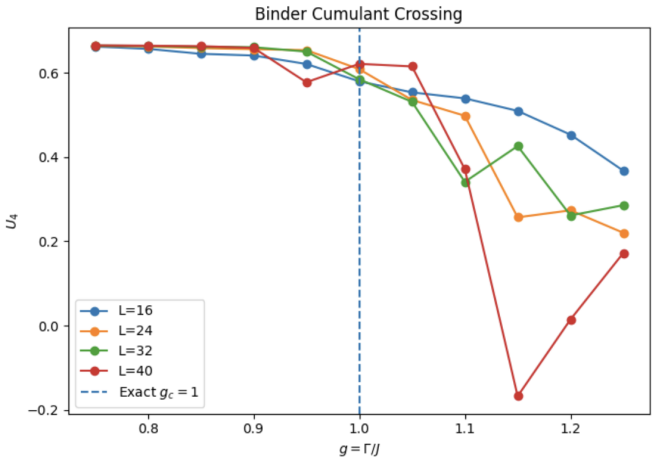


Fig. 4: Binder cumulant as a function of the transverse-field strength $g = \Gamma/J$ for several system sizes. The vertical dashed line indicates the exact critical point $g_c = 1$. The curves exhibit a common crossing region near the expected transition, although finite-size effects and Monte Carlo fluctuations broaden the intersection.

Although the crossings are not perfectly sharp, all system sizes indicate a transition region consistent with the exact critical point

$$g_c = 1.$$

The observed broadening is expected for finite systems and is further amplified by critical slowing down associated with local Metropolis updates [7]. Near the critical point, correlation times increase substantially, making it more difficult to obtain statistically independent samples within a fixed computational budget.

Consequently, the Binder analysis should be interpreted as qualitative evidence for the location of the transition rather than as a high-precision determination of the critical coupling. Nevertheless, the results are fully consistent with the theoretical prediction obtained from both the exact solution of the transverse-field Ising chain and the quantum-to-classical mapping developed in Section 2.

Taken together with the magnetization and kink-density measurements, the Binder cumulants provide an independent confirmation that the critical region is centered near

$$g = 1.$$

This agreement strengthens the overall interpretation of the numerical data and supports the identification of the observed transition as the quantum critical point of the transverse-field Ising model.

D. Correlation Length and Critical Correlations

A defining feature of continuous phase transitions is the growth of correlations over increasingly large length scales. Near a critical point, fluctuations become correlated across much of the system, leading to an enhanced correlation length.

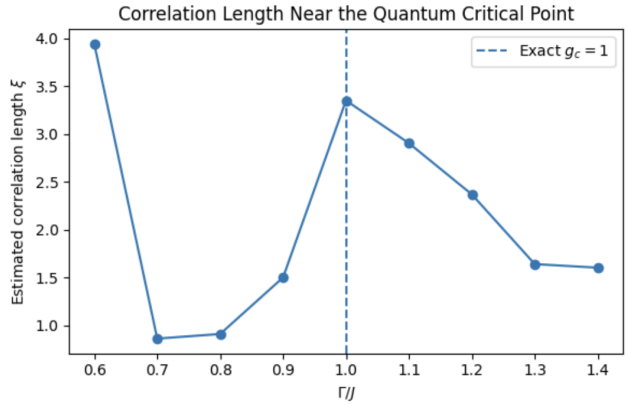


Fig. 5: Estimated finite-size correlation length as a function of the transverse-field strength $g = \Gamma/J$. The largest values occur near the critical region, indicating enhanced long-range correlations. The correlation lengths were obtained from simple exponential fits and should therefore be interpreted qualitatively rather than as precision measurements.

To investigate this behavior, spatial correlation functions were measured on the effective classical lattice and used to estimate a finite-size correlation length.

The connected correlation function was defined as

$$C(r) = \langle s_i s_{i+r} \rangle - \langle s_i \rangle^2,$$

where r denotes the spatial separation between spins. Away from criticality, correlations are expected to decay approximately exponentially,

$$C(r) \sim e^{-r/\xi},$$

allowing an estimate of the correlation length ξ to be obtained through numerical fitting.

Figure 5 shows the extracted correlation length as a function of the transverse-field strength.

The extracted correlation lengths exhibit a clear enhancement in the vicinity of

$$g \approx 1,$$

which is precisely where the other observables indicate the presence of a quantum phase transition. This behavior is consistent with the expected growth of correlations near criticality. Although the correlation length remains finite because the simulations were performed on finite lattices, the increase relative to both the ordered and disordered regimes provides additional evidence for critical behavior.

To better understand the underlying correlations, representative correlation functions are shown in Figure 6.

The correlation functions demonstrate that correlations persist over longer distances near

$$g \approx 1,$$

while more rapid decay is observed deeper within the disordered phase. This trend is consistent with the increase in

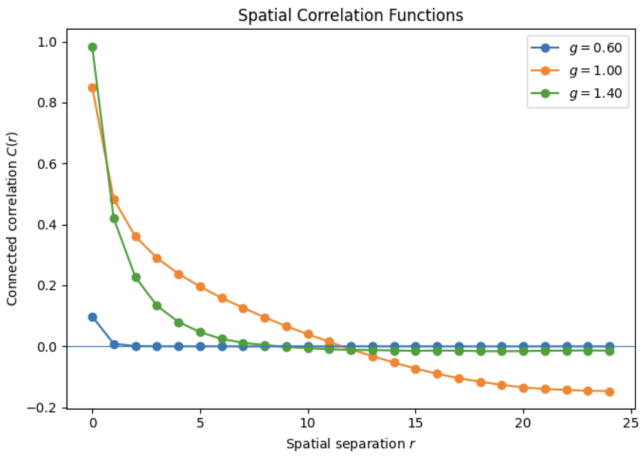


Fig. 6: Representative connected correlation functions for several values of the transverse-field strength. Correlations decay most slowly near the critical region, reflecting the growth of the correlation length.

the estimated correlation length and agrees qualitatively with the expected behavior of a system approaching a continuous phase transition.

It is important to emphasize that the correlation lengths reported here were obtained using simple exponential fits to finite-size data. In the ordered phase, the connected correlation function becomes small after subtraction of the magnetization contribution, making the fitting procedure sensitive to statistical fluctuations. Near criticality, finite-size effects and deviations from purely exponential behavior further limit the precision of the extracted values. Consequently, the reported correlation lengths should be interpreted as qualitative indicators of correlation growth rather than precise determinations of critical scaling.

Despite these limitations, the overall trend is clear. The largest correlation lengths occur near the same region where the magnetization decreases rapidly, the kink density increases, and the Binder cumulants cluster. The correlation analysis therefore provides an additional and independent signature of the quantum phase transition.

Taken together, the worldline configurations, magnetization measurements, Binder cumulants, kink densities, and correlation functions present a coherent picture of the transverse-field Ising transition. All observables consistently indicate a critical region centered near

$$g = 1,$$

in agreement with the exact solution of the model.

V. Discussion

A. Instantons as the Microscopic Mechanism of the Transition

The central objective of this project was to investigate whether the quantum phase transition of the transverse-field Ising model could be understood through the imaginary-time path integral formalism and, in particular, through the behavior of instantons. The numerical results strongly support this interpretation.

In the worldline representation, the transverse field generates spin flips along the imaginary-time direction. These spin flips appear as kinks in the worldlines and correspond to tunneling events between locally ordered spin configurations. Consequently, the density of kinks provides a direct measure of the strength of quantum fluctuations.

The numerical simulations reveal a clear relationship between instanton density and magnetic order. In the ferromagnetic phase,

$$g < 1,$$

worldlines remain largely coherent and only a small number of instantons are present. The magnetization remains close to unity, indicating robust long-range order. As the transverse field increases toward the critical point, the density of instantons rises significantly and the worldlines become increasingly fragmented. Simultaneously, the magnetization decreases and correlation lengths grow.

Beyond the critical region,

$$g > 1,$$

instantons become abundant throughout the spacetime lattice. The resulting tunneling activity destroys long-range ferromagnetic order and drives the system into the quantum paramagnetic phase. From the path-integral perspective, the quantum phase transition may therefore be interpreted as a transition from a regime of rare instantons to one in which instantons proliferate and dominate the system's behavior.

This interpretation provides a microscopic explanation for the transition that complements the conventional order-parameter description. Rather than viewing the critical point solely as the location where the magnetization vanishes, the worldline formulation reveals how quantum tunneling events accumulate and ultimately disrupt the ordered state.

B. Connection to Quantum Criticality

Several independent observables indicate the presence of a critical region centered near

$$g = 1.$$

The magnetization decreases rapidly near this value, the kink density increases substantially, Binder cumulants cluster near the expected critical coupling, and the estimated correlation length reaches its largest values in the same region. Although each observable is subject to finite-size effects and statistical uncertainty, their collective behavior is highly consistent.

The growth of the correlation length is particularly significant because it reflects the emergence of fluctuations over increasingly large length scales. In an infinite system, the correlation length diverges at a continuous phase transition. While such a divergence cannot be observed directly in finite simulations, the enhanced correlations observed near

$$g \approx 1$$

are consistent with the expected approach to criticality.

The Binder cumulant analysis provides additional support for this conclusion. Although the crossings are broadened by finite-size effects and the use of local Metropolis updates, the crossing region remains centered near the exact critical value. The Binder results therefore serve as an independent confirmation of the transition identified through the other observables.

Taken together, the numerical data indicate that the simulated system reproduces the expected qualitative features of the quantum critical point of the transverse-field Ising chain.

C. Universality and the Quantum–Classical Mapping

One of the most important theoretical results underlying this project is the correspondence between the one-dimensional quantum transverse-field Ising model and the two-dimensional classical Ising model. Through the Suzuki–Trotter decomposition, the original quantum problem is transformed into an anisotropic classical statistical system defined on a spacetime lattice.

This mapping implies that the quantum critical point belongs to the same universality class as the classical two-dimensional Ising model [1, 4, 5]. Consequently, both systems share the same long-wavelength critical behavior despite their different microscopic descriptions.

The present simulations were not designed to perform a high-precision extraction of critical exponents. Achieving such accuracy would require substantially larger system sizes, improved statistics, and more sophisticated update algorithms. Nevertheless, the observed behavior is consistent with the expected phenomenology of the two-dimensional Ising universality class. The presence of a well-defined critical region, enhanced correlation lengths, and finite-size Binder crossings all support this interpretation.

More broadly, the quantum-to-classical mapping illustrates one of the central ideas of modern condensed matter physics: seemingly different systems can exhibit identical large-scale behavior near criticality. The emergence of universal behavior allows complex quantum phase transitions to be studied using classical statistical mechanics techniques, providing both conceptual insight and practical computational tools.

D. Limitations and Future Directions

Several limitations of the present study should be acknowledged.

First, all simulations were performed using local Metropolis updates. Near the critical point, such algorithms suffer from critical slowing down, leading to long autocorrelation times and increased statistical uncertainty. Cluster algorithms, such as the Wolff algorithm, would substantially improve sampling efficiency and produce more precise Binder crossings and correlation-length estimates [6].

Second, the correlation lengths reported in this work were extracted from simple exponential fits to finite-size data. These estimates provide useful qualitative information regarding the growth of correlations near the transition, but they should not be interpreted as precision measurements of critical scaling.

Finally, the system sizes considered here remain modest by modern Monte Carlo standards. Larger lattices would allow more reliable finite-size scaling analyses and could be used to extract critical exponents directly.

Despite these limitations, the simulations successfully reproduce the principal qualitative features of the transverse-field Ising transition and provide a clear physical picture of how quantum fluctuations drive the destruction of long-range order.

VI. Conclusion

In this project, the quantum phase transition of the one-dimensional transverse-field Ising model was investigated using the imaginary-time path integral formalism and classical Monte Carlo simulation. Beginning from the quantum Hamiltonian, the Suzuki–Trotter decomposition was used to map the system onto an anisotropic two-dimensional classical Ising model defined on a spacetime lattice. This mapping transformed the original quantum problem into a form that could be studied using standard statistical-mechanics techniques while preserving the critical properties of the underlying quantum system.

The worldline representation provided a particularly intuitive picture of quantum fluctuations. In this formulation, tunneling events generated by the transverse field appear as kinks, or instantons, along the imaginary-time direction. By analyzing worldline configurations across the phase diagram, it was possible to directly visualize the evolution of the system from an ordered ferromagnetic state to a disordered quantum paramagnet.

Monte Carlo simulations were used to measure the magnetization, kink density, Binder cumulant, and correlation functions of the effective classical model. These observables consistently identified a critical region centered near

$$g = \frac{\Gamma}{J} = 1,$$

in agreement with the exact solution of the transverse-field Ising chain. As the critical point was approached, the magnetization decreased, the correlation length increased, and the density of instantons rose significantly. The Binder cumulant analysis provided additional finite-size evidence for the location of the transition.

The most important physical result of this work is the demonstration that the quantum phase transition can be understood as the proliferation of instantons in imaginary time. In the ordered phase, worldlines remain largely coherent and tunneling events are rare. As the transverse field increases, instantons become increasingly common and eventually disrupt long-range ferromagnetic order. From the perspective of the path-integral formulation, the transition is therefore not simply characterized by the disappearance of the order parameter, but by a fundamental change in the structure of worldline configurations.

More broadly, this project illustrates the power of the quantum-to-classical correspondence. Through the Suzuki–Trotter mapping, a quantum many-body problem was reformulated as a classical statistical system, making it possible to investigate quantum critical phenomena using computational techniques originally developed for classical models. The resulting connection between worldlines, instantons, universality, and critical behavior provides a concrete example of how path-integral methods offer both conceptual insight and practical tools for the study of quantum phase transitions.

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APPENDIX A
SIMULATION NOTEBOOK

The full Python notebook used to generate and simulate the Monte Carlo data and figures is included below.

In [3]:
```python
import numpy as np
import matplotlib.pyplot as plt
from dataclasses import dataclass

@dataclass
class TFIMParams:
    """
    Parameters for the Suzuki-Trotter mapped 2D classical Ising model.

    We set J = 1 by default, so g = Gamma/J = Gamma.
    The imaginary-time step is delta_tau = beta / M.
    """
    N: int              # spatial size
    M: int              # imaginary-time slices
    g: float            # g = Gamma / J
    J: float = 1.0
    delta_tau: float = 0.25


def couplings(params: TFIMParams):
    """
    Return spatial and imaginary-time couplings:
        K_s = J delta_tau
        K_tau = (1/2) ln coth(Gamma delta_tau)

    Avoid g = 0 exactly because K_tau -> infinity.
    """
    Gamma = params.g * params.J
    a = Gamma * params.delta_tau

    if a <= 0:
        raise ValueError("Gamma * delta_tau must be positive. Use small nonz

    K_s = params.J * params.delta_tau
    K_tau = 0.5 * np.log(1.0 / np.tanh(a))  # ln(coth a)

    return K_s, K_tau
```

In [4]:
```python
def initialize_lattice(N, M, ordered=False, rng=None):
    """
    Create an N x M Ising worldline lattice.

    N: spatial sites
    M: imaginary-time slices
    ordered=False gives random spins.
    ordered=True gives all +1 spins.
    """
    if rng is None:
        rng = np.random.default_rng()

    if ordered:
        return np.ones((N, M), dtype=np.int8)

    return rng.choice([-1, 1], size=(N, M)).astype(np.int8)
```

```
def delta_energy_flip(spins, i, t, K_s, K_tau):
    """
    Compute classical energy change for flipping spin s_{i,t}.

    E_cl =
        -K_s sum s_{i,t} s_{i+1,t}
        -K_tau sum s_{i,t} s_{i,t+1}

    Periodic boundary conditions are used in both directions.
    """
    N, M = spins.shape
    s = spins[i, t]

    spatial_neighbors = spins[(i + 1) % N, t] + spins[(i - 1) % N, t]
    time_neighbors = spins[i, (t + 1) % M] + spins[i, (t - 1) % M]

    dE = 2 * s * (K_s * spatial_neighbors + K_tau * time_neighbors)

    return dE
```

In [5]:

```
def metropolis_sweep(spins, K_s, K_tau, rng=None):
    """
    Perform one full Metropolis sweep.

    One sweep = N*M attempted spin flips.
    """
    if rng is None:
        rng = np.random.default_rng()

    N, M = spins.shape
    accepted = 0
    total = N * M

    for _ in range(total):
        i = rng.integers(0, N)
        t = rng.integers(0, M)

        dE = delta_energy_flip(spins, i, t, K_s, K_tau)

        if dE <= 0 or rng.random() < np.exp(-dE):
            spins[i, t] *= -1
            accepted += 1

    return accepted / total
```

In [6]:

```
def magnetization(spins):
    """
    Spacetime-averaged magnetization for one configuration.
    """
    return np.mean(spins)


def abs_magnetization(spins):
```

```
    """
    Absolute magnetization, useful because finite simulations can tunnel
    between + and - ordered sectors.
    """
    return abs(magnetization(spins))


def kink_density(spins):
    """
    Temporal kink/instanton density:

        n_kink = (1/NM) sum_{i,t} (1 - s_{i,t} s_{i,t+1}) / 2

    Counts spin flips along imaginary time.
    """
    shifted = np.roll(spins, shift=-1, axis=1)
    return np.mean((1 - spins * shifted) / 2)


def classical_energy_density(spins, K_s, K_tau):
    """
    Classical energy per spacetime site.
    """
    spatial = np.sum(spins * np.roll(spins, shift=-1, axis=0))
    temporal = np.sum(spins * np.roll(spins, shift=-1, axis=1))

    E = -K_s * spatial - K_tau * temporal
    return E / spins.size


def binder_cumulant(m_samples):
    """
    Binder cumulant:
        U4 = 1 - <m^4> / (3 <m^2>^2)
    """
    m_samples = np.asarray(m_samples)
    m2 = np.mean(m_samples**2)
    m4 = np.mean(m_samples**4)

    if m2 == 0:
        return np.nan

    return 1 - m4 / (3 * m2**2)
```

In [7]:

```
def run_simulation(
    params: TFIMParams,
    n_therm=1000,
    n_measure=3000,
    measure_every=5,
    ordered_start=False,
    seed=1234
):
    """
    Run Metropolis Monte Carlo for one value of g = Gamma/J.

    Returns:
```

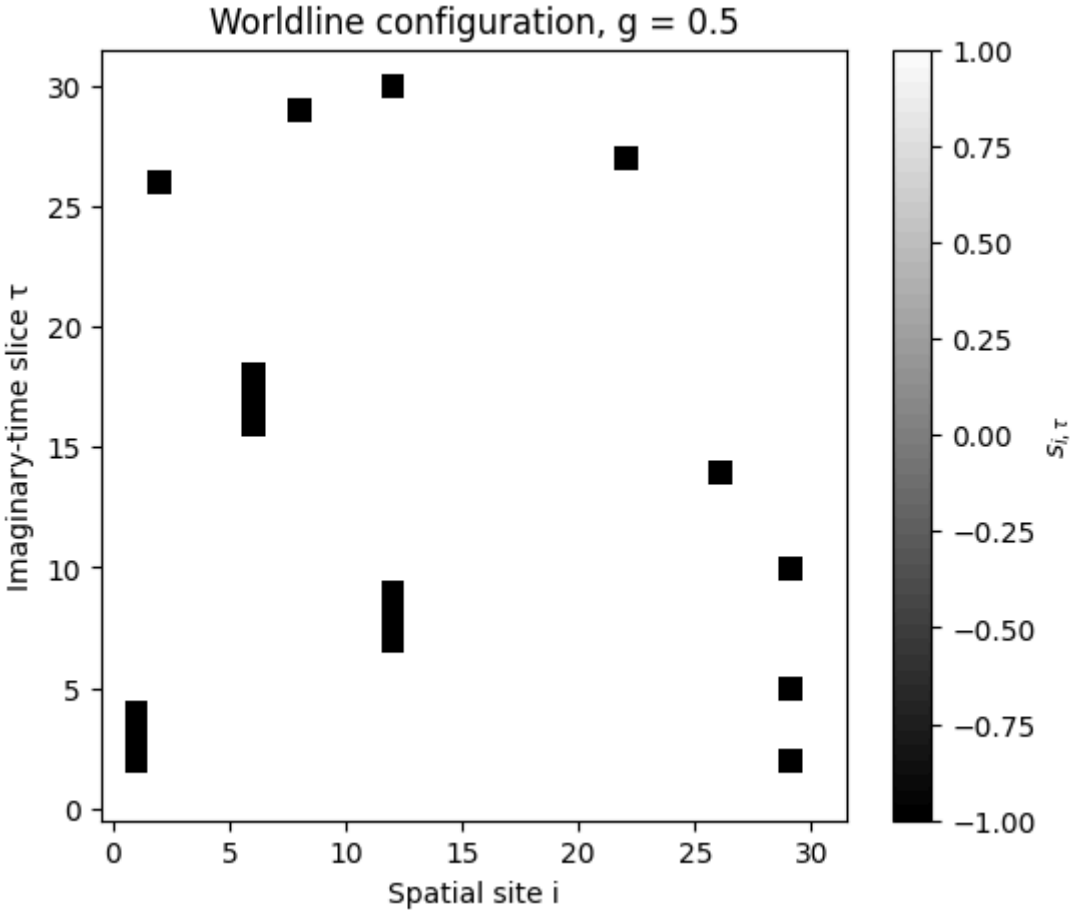
```
    results dictionary
    final spin configuration
"""
rng = np.random.default_rng(seed)

K_s, K_tau = couplings(params)
spins = initialize_lattice(params.N, params.M, ordered=ordered_start, rr

# Thermalization
accept_rates_therm = []
for _ in range(n_therm):
    acc = metropolis_sweep(spins, K_s, K_tau, rng)
    accept_rates_therm.append(acc)

# Measurements
m_samples = []
abs_m_samples = []
kink_samples = []
energy_samples = []
accept_rates_meas = []

for sweep in range(n_measure):
    acc = metropolis_sweep(spins, K_s, K_tau, rng)

    if sweep % measure_every == 0:
        m = magnetization(spins)
        m_samples.append(m)
        abs_m_samples.append(abs(m))
        kink_samples.append(kink_density(spins))
        energy_samples.append(classical_energy_density(spins, K_s, K_tau
        accept_rates_meas.append(acc)

m_samples = np.array(m_samples)
abs_m_samples = np.array(abs_m_samples)
kink_samples = np.array(kink_samples)
energy_samples = np.array(energy_samples)

results = {
    "g": params.g,
    "K_s": K_s,
    "K_tau": K_tau,
    "m_abs_mean": np.mean(abs_m_samples),
    "m_abs_err": np.std(abs_m_samples) / np.sqrt(len(abs_m_samples)),
    "m_mean": np.mean(m_samples),
    "kink_mean": np.mean(kink_samples),
    "kink_err": np.std(kink_samples) / np.sqrt(len(kink_samples)),
    "energy_mean": np.mean(energy_samples),
    "energy_err": np.std(energy_samples) / np.sqrt(len(energy_samples)),
    "binder": binder_cumulant(m_samples),
    "acceptance_therm": np.mean(accept_rates_therm),
    "acceptance_meas": np.mean(accept_rates_meas),
    "m_samples": m_samples,
    "kink_samples": kink_samples,
    "energy_samples": energy_samples,
}
```

```
    return results, spins
```

In [8]:
```
params = TFIMParams(
    N=32,
    M=32,
    g=0.5,
    J=1.0,
    delta_tau=0.25
)

results, spins = run_simulation(
    params,
    n_therm=500,
    n_measure=1000,
    measure_every=5,
    ordered_start=True,
    seed=1
)

for key, value in results.items():
    if not isinstance(value, np.ndarray):
        print(f"{key}: {value}")
```

```
g: 0.5
K_s: 0.25
K_tau: 1.0423154846624378
m_abs_mean: 0.9660546875
m_abs_err: 0.0010593394225681546
m_mean: 0.9660546875
kink_mean: 0.01970703125
kink_err: 0.0004828190577780779
energy_mean: -1.235662307942735
energy_err: 0.0014080512516824904
binder: 0.6663498769135048
acceptance_therm: 0.025671875
acceptance_meas: 0.0283203125
```

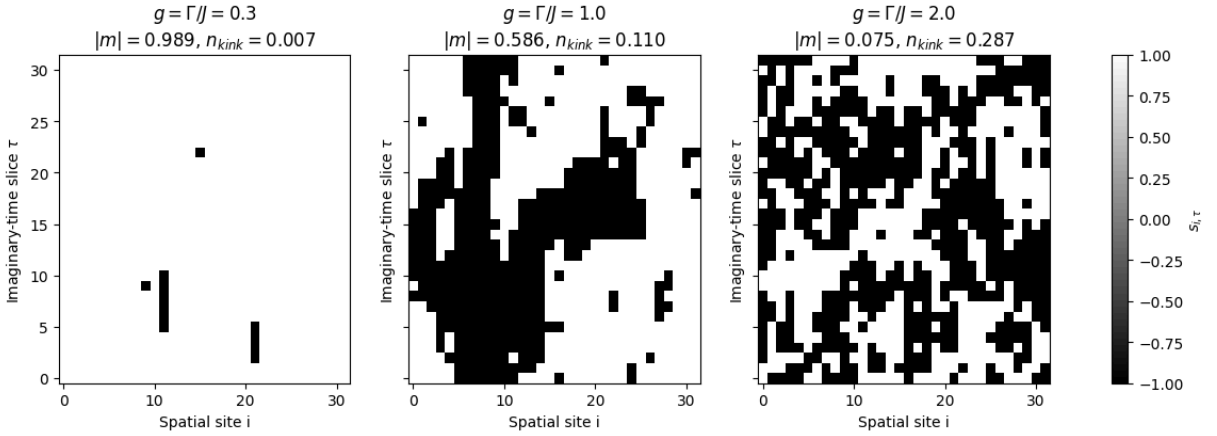
In [9]:
```
plt.figure(figsize=(6, 5))
plt.imshow(spins.T, aspect="auto", origin="lower", cmap="gray")
plt.xlabel("Spatial site i")
plt.ylabel("Imaginary-time slice τ")
plt.title(f"Worldline configuration, g = {params.g}")
plt.colorbar(label=r"$s_{i,\tau}$")
plt.show()
```



In [10]:
```
def quick_visual_tests(
    g_values=(0.3, 1.0, 2.0),
    N=32,
    M=32,
    delta_tau=0.25,
    n_therm=1000,
    n_measure=1500,
    measure_every=5,
    seed_base=100
):
    """
    Run quick simulations at several g values and plot final worldline confi
    """

    final_results = []

    fig, axes = plt.subplots(1, len(g_values), figsize=(5 * len(g_values), 4

    if len(g_values) == 1:
        axes = [axes]

    for ax, g in zip(axes, g_values):
        params = TFIMParams(
            N=N,
            M=M,
            g=g,
            J=1.0,
```

```
            delta_tau=delta_tau
        )

        results, spins = run_simulation(
            params,
            n_therm=n_therm,
            n_measure=n_measure,
            measure_every=measure_every,
            ordered_start=True,
            seed=seed_base + int(100 * g)
        )

        final_results.append(results)

        im = ax.imshow(spins.T, aspect="auto", origin="lower", cmap="gray",
        ax.set_title(
            rf"$g=\Gamma/J={g}$" + "\n"
            + rf"$|m|={results['m_abs_mean']:.3f}$, "
            + rf"$n_{{kink}}={results['kink_mean']:.3f}$"
        )
        ax.set_xlabel("Spatial site i")
        ax.set_ylabel(r"Imaginary-time slice $\tau$")

    fig.colorbar(im, ax=axes, label=r"$s_{i,\tau}$")
    plt.show()

    return final_results
```

In [11]:
```
quick_results = quick_visual_tests()
```



In [12]:
```
for r in quick_results:
    print(
        f"g={r['g']:.2f} | "
        f"K_s={r['K_s']:.3f} | "
        f"K_tau={r['K_tau']:.3f} | "
        f"|m|={r['m_abs_mean']:.3f} ± {r['m_abs_err']:.3f} | "
        f"kink={r['kink_mean']:.3f} ± {r['kink_err']:.3f} | "
        f"Binder={r['binder']:.3f} | "
        f"accept={r['acceptance_meas']:.3f}"
        )
```

```
g=0.30 | K_s=0.250 | K_tau=1.296 | |m|=0.989 ± 0.000 | kink=0.007 ± 0.000 |
Binder=0.667 | accept=0.010
g=1.00 | K_s=0.250 | K_tau=0.703 | |m|=0.586 ± 0.011 | kink=0.110 ± 0.001 |
Binder=0.564 | accept=0.173
g=2.00 | K_s=0.250 | K_tau=0.386 | |m|=0.075 ± 0.003 | kink=0.287 ± 0.001 |
Binder=-0.100 | accept=0.476
```

In [13]:

```python
# PARAMETER SWEEP

g_values = np.linspace(0.2, 2.0, 19)

sweep_results = {
    "g": [],
    "m": [],
    "m_err": [],
    "kink": [],
    "kink_err": [],
    "energy": [],
    "energy_err": [],
    "binder": [],
    "acceptance": []
}

for idx, g in enumerate(g_values):

    params = TFIMParams(
        N=32,
        M=32,
        g=float(g),
        J=1.0,
        delta_tau=0.25
    )

    out, final_spins = run_simulation(
        params,
        n_therm=3000,
        n_measure=5000,
        measure_every=5,
        ordered_start=True,
        seed=1000 + idx
    )

    sweep_results["g"].append(g)
    sweep_results["m"].append(out["m_abs_mean"])
    sweep_results["m_err"].append(out["m_abs_err"])
    sweep_results["kink"].append(out["kink_mean"])
    sweep_results["kink_err"].append(out["kink_err"])
    sweep_results["energy"].append(out["energy_mean"])
    sweep_results["energy_err"].append(out["energy_err"])
    sweep_results["binder"].append(out["binder"])
    sweep_results["acceptance"].append(out["acceptance_meas"])

    print(
        f"g={g:.2f}"
        f" | K_s={out['K_s']:.3f}"
        f" | K_tau={out['K_tau']:.3f}"
```

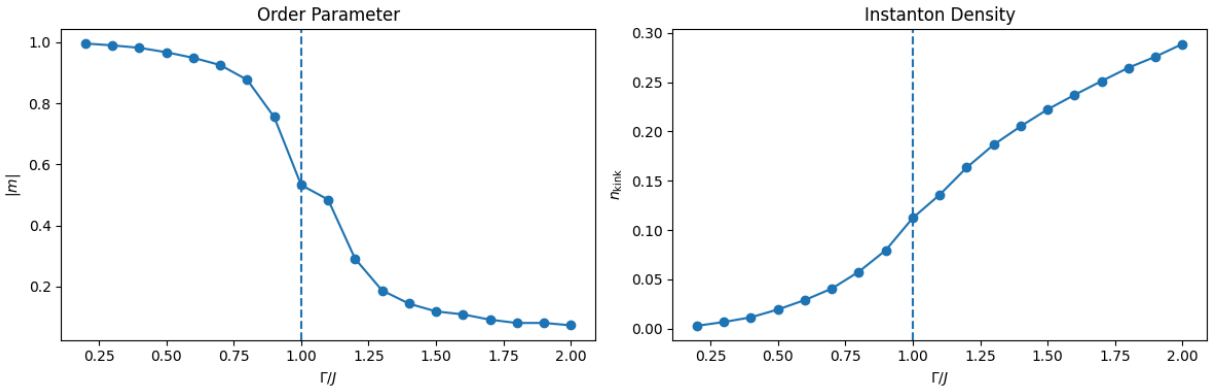
```
        f" | |m|={out['m_abs_mean']:.3f}"
        f" | kink={out['kink_mean']:.3f}"
        f" | U4={out['binder']:.3f}"
        f" | acc={out['acceptance_meas']:.3f}"
    )
```

```
g=0.20 | K_s=0.250 | K_tau=1.498 | |m|=0.995 | kink=0.003 | U4=0.667 | acc=
0.004
g=0.30 | K_s=0.250 | K_tau=1.296 | |m|=0.989 | kink=0.007 | U4=0.667 | acc=
0.009
g=0.40 | K_s=0.250 | K_tau=1.153 | |m|=0.981 | kink=0.011 | U4=0.667 | acc=
0.016
g=0.50 | K_s=0.250 | K_tau=1.042 | |m|=0.967 | kink=0.019 | U4=0.666 | acc=
0.027
g=0.60 | K_s=0.250 | K_tau=0.952 | |m|=0.949 | kink=0.029 | U4=0.666 | acc=
0.041
g=0.70 | K_s=0.250 | K_tau=0.877 | |m|=0.925 | kink=0.041 | U4=0.666 | acc=
0.060
g=0.80 | K_s=0.250 | K_tau=0.811 | |m|=0.876 | kink=0.058 | U4=0.663 | acc=
0.085
g=0.90 | K_s=0.250 | K_tau=0.754 | |m|=0.755 | kink=0.080 | U4=0.627 | acc=
0.121
g=1.00 | K_s=0.250 | K_tau=0.703 | |m|=0.532 | kink=0.112 | U4=0.512 | acc=
0.175
g=1.10 | K_s=0.250 | K_tau=0.658 | |m|=0.485 | kink=0.136 | U4=0.528 | acc=
0.215
g=1.20 | K_s=0.250 | K_tau=0.617 | |m|=0.291 | kink=0.163 | U4=0.343 | acc=
0.262
g=1.30 | K_s=0.250 | K_tau=0.579 | |m|=0.188 | kink=0.187 | U4=0.216 | acc=
0.301
g=1.40 | K_s=0.250 | K_tau=0.545 | |m|=0.144 | kink=0.205 | U4=0.029 | acc=
0.334
g=1.50 | K_s=0.250 | K_tau=0.513 | |m|=0.119 | kink=0.222 | U4=0.077 | acc=
0.362
g=1.60 | K_s=0.250 | K_tau=0.484 | |m|=0.109 | kink=0.237 | U4=0.029 | acc=
0.388
g=1.70 | K_s=0.250 | K_tau=0.457 | |m|=0.092 | kink=0.251 | U4=0.103 | acc=
0.413
g=1.80 | K_s=0.250 | K_tau=0.431 | |m|=0.081 | kink=0.265 | U4=0.042 | acc=
0.436
g=1.90 | K_s=0.250 | K_tau=0.408 | |m|=0.081 | kink=0.276 | U4=-0.022 | acc=
0.456
g=2.00 | K_s=0.250 | K_tau=0.386 | |m|=0.073 | kink=0.289 | U4=-0.019 | acc=
0.477
```

In [14]:

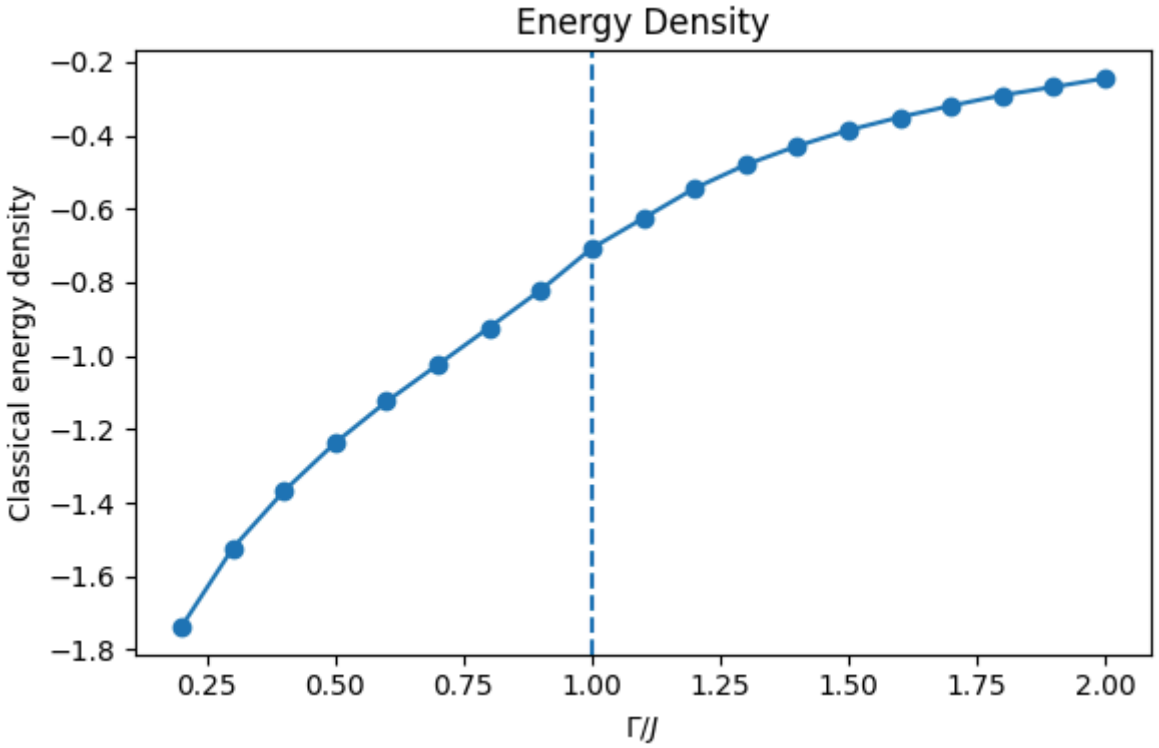
```
fig, ax = plt.subplots(1, 2, figsize=(12, 4))

ax[0].errorbar(
    sweep_results["g"],
    sweep_results["m"],
    yerr=sweep_results["m_err"],
    marker="o",
    capsize=3
)
ax[0].axvline(1.0, linestyle="--")
ax[0].set_xlabel(r"$\Gamma/J$")
```

```
ax[0].set_ylabel(r"$|m|$")
ax[0].set_title("Order Parameter")

ax[1].errorbar(
    sweep_results["g"],
    sweep_results["kink"],
    yerr=sweep_results["kink_err"],
    marker="o",
    capsize=3
)
ax[1].axvline(1.0, linestyle="--")
ax[1].set_xlabel(r"$\Gamma/J$")
ax[1].set_ylabel(r"$n_{\rm kink}$")
ax[1].set_title("Instanton Density")

plt.tight_layout()
plt.show()
```

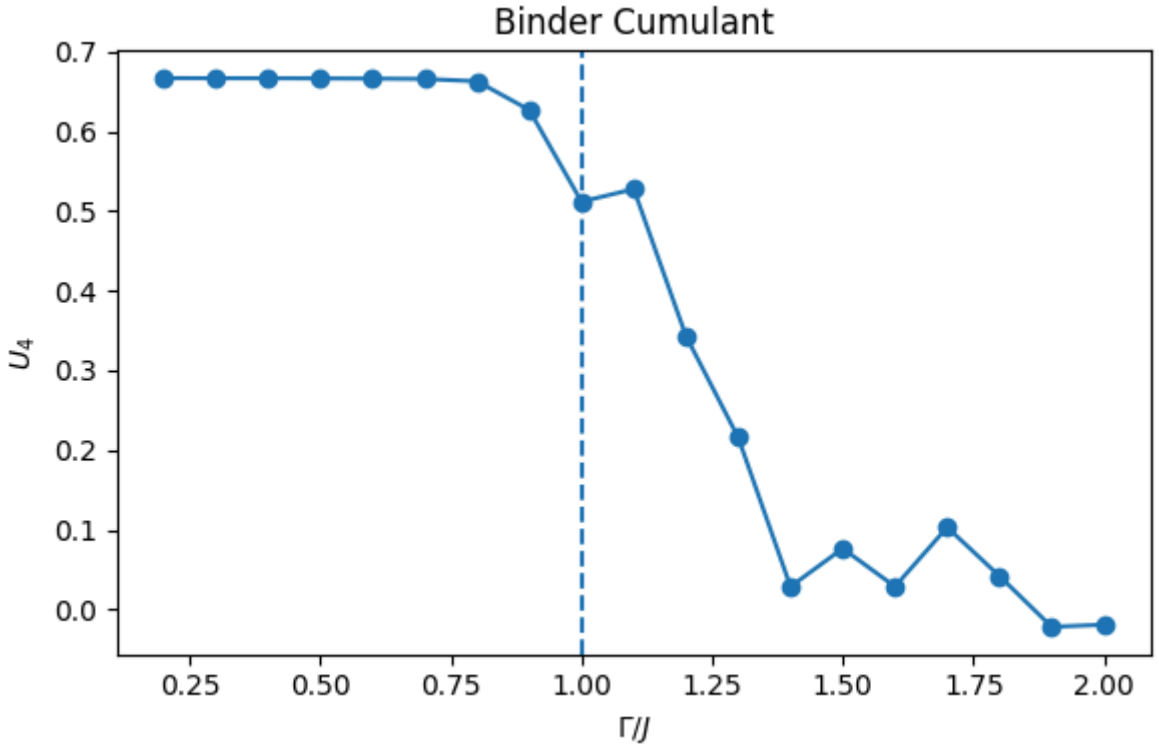


In [15]:

```
plt.figure(figsize=(6, 4))

plt.errorbar(
    sweep_results["g"],
    sweep_results["energy"],
    yerr=sweep_results["energy_err"],
    marker="o",
    capsize=3
)
plt.axvline(1.0, linestyle="--")
plt.xlabel(r"$\Gamma/J$")
plt.ylabel("Classical energy density")
plt.title("Energy Density")
plt.tight_layout()
plt.show()
```



In [16]:
```
plt.figure(figsize=(6, 4))

plt.plot(
    sweep_results["g"],
    sweep_results["binder"],
    marker="o"
)
plt.axvline(1.0, linestyle="--")
plt.xlabel(r"$\Gamma/J$")
plt.ylabel(r"$U_4$")
plt.title("Binder Cumulant")
plt.tight_layout()
plt.show()
```



In [17]:

```python
# ============================================================
# MULTI-SIZE BINDER CUMULANT SWEEP
# ============================================================

def binder_size_sweep(
    sizes=(16, 24, 32, 40),
    g_values=np.linspace(0.7, 1.3, 13),
    delta_tau=0.25,
    n_therm=3000,
    n_measure=5000,
    measure_every=5,
    seed_base=5000
):
    """
    Run Binder cumulant sweeps for several square spacetime lattices N=M=L.

    This is used to locate the critical point via Binder crossing.
    """

    binder_data = {}

    for size_idx, L in enumerate(sizes):
        print(f"\nRunning size L = {L}")

        binder_data[L] = {
            "g": [],
            "binder": [],
            "m": [],
            "kink": [],
            "acceptance": []
        }
```

```
        for g_idx, g in enumerate(g_values):
            params = TFIMParams(
                N=L,
                M=L,
                g=float(g),
                J=1.0,
                delta_tau=delta_tau
            )

            out, _ = run_simulation(
                params,
                n_therm=n_therm,
                n_measure=n_measure,
                measure_every=measure_every,
                ordered_start=True,
                seed=seed_base + 1000 * size_idx + g_idx
            )

            binder_data[L]["g"].append(float(g))
            binder_data[L]["binder"].append(out["binder"])
            binder_data[L]["m"].append(out["m_abs_mean"])
            binder_data[L]["kink"].append(out["kink_mean"])
            binder_data[L]["acceptance"].append(out["acceptance_meas"])

            print(
                f"L={L:2d} | g={g:.3f} | "
                f"U4={out['binder']:.3f} | "
                f"|m|={out['m_abs_mean']:.3f} | "
                f"kink={out['kink_mean']:.3f} | "
                f"acc={out['acceptance_meas']:.3f}"
            )

    return binder_data
```

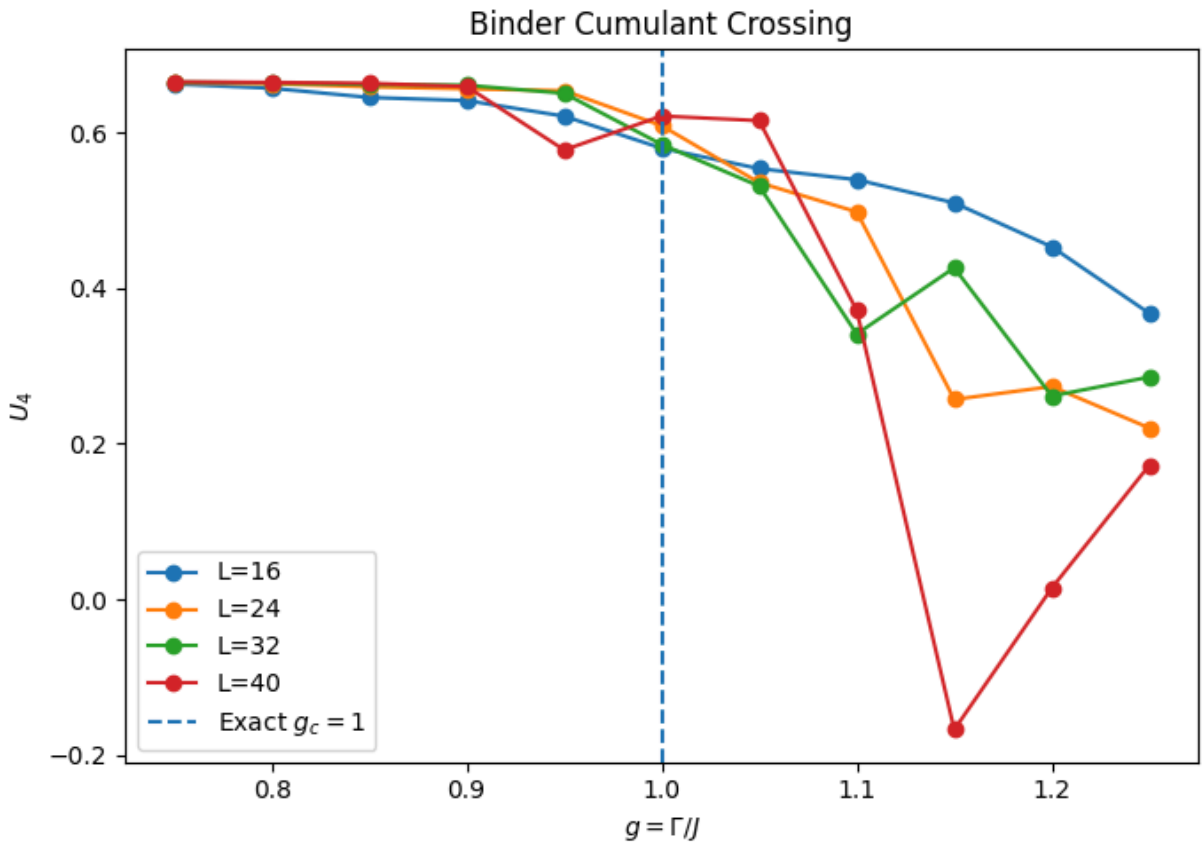
In [18]:

```
g_binder = np.linspace(0.75, 1.25, 11)

binder_data = binder_size_sweep(
    sizes=(16, 24, 32, 40),
    g_values=g_binder,
    delta_tau=0.25,
    n_therm=3000,
    n_measure=5000,
    measure_every=5,
    seed_base=9000
)
```

```
Running size L = 16
L=16 | g=0.750 | U4=0.663 | |m|=0.916 | kink=0.047 | acc=0.068
L=16 | g=0.800 | U4=0.657 | |m|=0.886 | kink=0.056 | acc=0.083
L=16 | g=0.850 | U4=0.646 | |m|=0.833 | kink=0.069 | acc=0.104
L=16 | g=0.900 | U4=0.642 | |m|=0.815 | kink=0.077 | acc=0.117
L=16 | g=0.950 | U4=0.622 | |m|=0.765 | kink=0.088 | acc=0.134
L=16 | g=1.000 | U4=0.580 | |m|=0.672 | kink=0.106 | acc=0.164
L=16 | g=1.050 | U4=0.554 | |m|=0.617 | kink=0.117 | acc=0.185
L=16 | g=1.100 | U4=0.540 | |m|=0.581 | kink=0.128 | acc=0.202
L=16 | g=1.150 | U4=0.510 | |m|=0.543 | kink=0.136 | acc=0.217
L=16 | g=1.200 | U4=0.453 | |m|=0.463 | kink=0.158 | acc=0.251
L=16 | g=1.250 | U4=0.368 | |m|=0.388 | kink=0.171 | acc=0.275

Running size L = 24
L=24 | g=0.750 | U4=0.664 | |m|=0.908 | kink=0.048 | acc=0.070
L=24 | g=0.800 | U4=0.663 | |m|=0.892 | kink=0.055 | acc=0.081
L=24 | g=0.850 | U4=0.659 | |m|=0.855 | kink=0.066 | acc=0.099
L=24 | g=0.900 | U4=0.657 | |m|=0.831 | kink=0.075 | acc=0.113
L=24 | g=0.950 | U4=0.654 | |m|=0.803 | kink=0.085 | acc=0.129
L=24 | g=1.000 | U4=0.609 | |m|=0.681 | kink=0.104 | acc=0.161
L=24 | g=1.050 | U4=0.536 | |m|=0.563 | kink=0.121 | acc=0.188
L=24 | g=1.100 | U4=0.498 | |m|=0.489 | kink=0.134 | acc=0.211
L=24 | g=1.150 | U4=0.257 | |m|=0.318 | kink=0.154 | acc=0.245
L=24 | g=1.200 | U4=0.274 | |m|=0.315 | kink=0.164 | acc=0.262
L=24 | g=1.250 | U4=0.220 | |m|=0.250 | kink=0.178 | acc=0.285

Running size L = 32
L=32 | g=0.750 | U4=0.665 | |m|=0.908 | kink=0.048 | acc=0.070
L=32 | g=0.800 | U4=0.664 | |m|=0.889 | kink=0.055 | acc=0.082
L=32 | g=0.850 | U4=0.662 | |m|=0.860 | kink=0.065 | acc=0.097
L=32 | g=0.900 | U4=0.661 | |m|=0.835 | kink=0.074 | acc=0.111
L=32 | g=0.950 | U4=0.651 | |m|=0.778 | kink=0.088 | acc=0.133
L=32 | g=1.000 | U4=0.585 | |m|=0.627 | kink=0.105 | acc=0.162
L=32 | g=1.050 | U4=0.532 | |m|=0.521 | kink=0.124 | acc=0.195
L=32 | g=1.100 | U4=0.341 | |m|=0.344 | kink=0.141 | acc=0.224
L=32 | g=1.150 | U4=0.426 | |m|=0.365 | kink=0.150 | acc=0.239
L=32 | g=1.200 | U4=0.261 | |m|=0.277 | kink=0.164 | acc=0.263
L=32 | g=1.250 | U4=0.286 | |m|=0.264 | kink=0.173 | acc=0.279

Running size L = 40
L=40 | g=0.750 | U4=0.666 | |m|=0.909 | kink=0.048 | acc=0.069
L=40 | g=0.800 | U4=0.665 | |m|=0.886 | kink=0.056 | acc=0.083
L=40 | g=0.850 | U4=0.664 | |m|=0.856 | kink=0.066 | acc=0.099
L=40 | g=0.900 | U4=0.660 | |m|=0.818 | kink=0.077 | acc=0.116
L=40 | g=0.950 | U4=0.578 | |m|=0.648 | kink=0.092 | acc=0.142
L=40 | g=1.000 | U4=0.622 | |m|=0.666 | kink=0.104 | acc=0.162
L=40 | g=1.050 | U4=0.616 | |m|=0.588 | kink=0.120 | acc=0.187
L=40 | g=1.100 | U4=0.372 | |m|=0.341 | kink=0.141 | acc=0.224
L=40 | g=1.150 | U4=-0.168 | |m|=0.182 | kink=0.157 | acc=0.251
L=40 | g=1.200 | U4=0.014 | |m|=0.158 | kink=0.167 | acc=0.267
L=40 | g=1.250 | U4=0.172 | |m|=0.191 | kink=0.176 | acc=0.284
```

In [19]:
```
# ============================================================
# PLOT BINDER CROSSING
# ============================================================
```

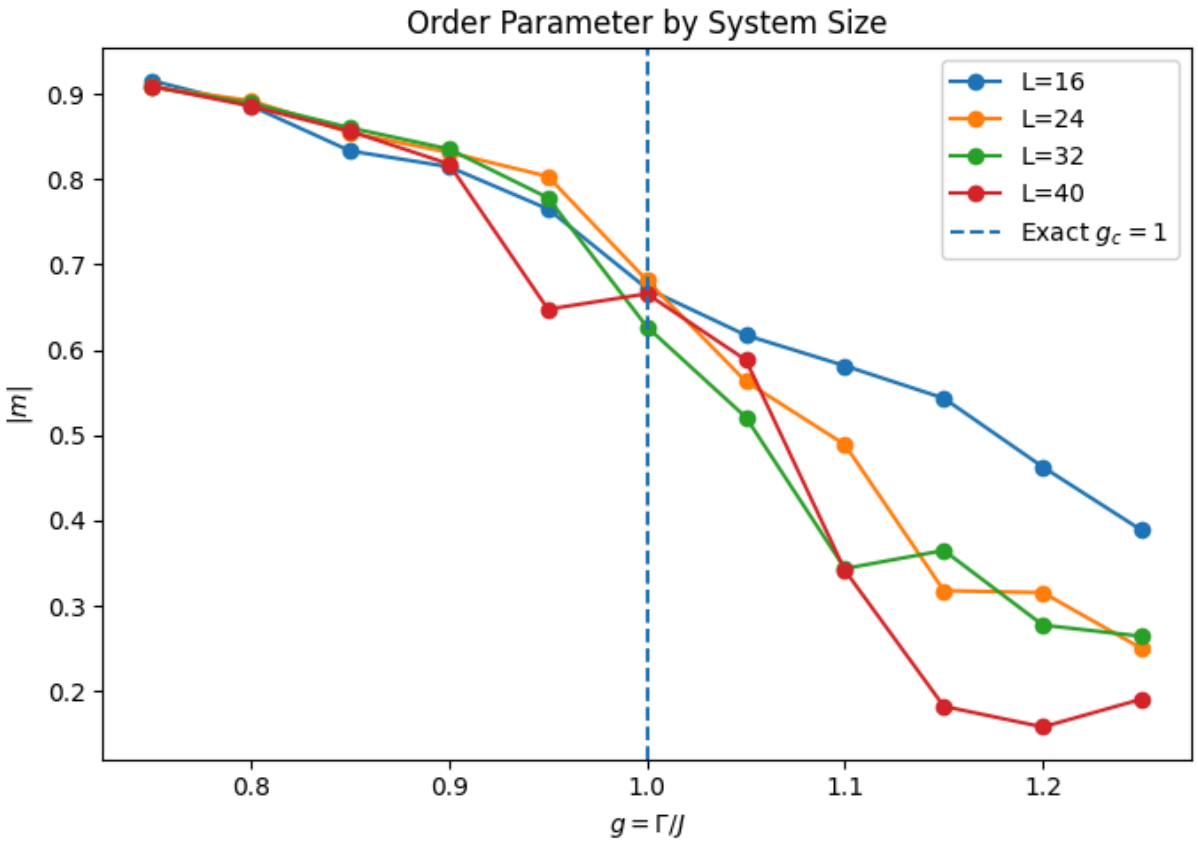
```
plt.figure(figsize=(7, 5))

for L, data in binder_data.items():
    plt.plot(
        data["g"],
        data["binder"],
        marker="o",
        label=f"L={L}"
    )

plt.axvline(1.0, linestyle="--", label=r"Exact $g_c=1$")
plt.xlabel(r"$g=\Gamma/J$")
plt.ylabel(r"$U_4$")
plt.title("Binder Cumulant Crossing")
plt.legend()
plt.tight_layout()
plt.show()
```



In [20]:

```
# ============================================================
# MAGNETIZATION BY SIZE
# ============================================================

plt.figure(figsize=(7, 5))

for L, data in binder_data.items():
    plt.plot(
        data["g"],
        data["m"],
        marker="o",
        label=f"L={L}"
```

```
    )

plt.axvline(1.0, linestyle="--", label=r"Exact $g_c=1$")
plt.xlabel(r"$g=\Gamma/J$")
plt.ylabel(r"$|m|$")
plt.title("Order Parameter by System Size")
plt.legend()
plt.tight_layout()
plt.show()
```



In [21]:

```
def spatial_correlation(spins):
    """
    Compute equal-imaginary-time spatial correlation function:

        C(r) = <s_{i,t} s_{i+r,t}> - <m>^2

    averaged over all spatial sites i and imaginary-time slices t.

    Returns:
        r_values, C_connected
    """
    N, M = spins.shape

    m = np.mean(spins)
    r_values = np.arange(N // 2 + 1)

    C = []

    for r in r_values:
        shifted = np.roll(spins, shift=-r, axis=0)
```

```
        corr_r = np.mean(spins * shifted)
        C.append(corr_r - m**2)

    return r_values, np.array(C)


def estimate_correlation_length(r_values, C_values, r_min=1, r_max=None):
    """
    Estimate correlation length by fitting:

        C(r) ~ A exp(-r/xi)

    so

        log C(r) = log A - r/xi.

    We only fit positive C(r), excluding r=0.
    """
    if r_max is None:
        r_max = len(r_values) - 1

    r = np.asarray(r_values)
    C = np.asarray(C_values)

    mask = (
        (r >= r_min)
        & (r <= r_max)
        & (C > 0)
        & np.isfinite(C)
    )

    r_fit = r[mask]
    C_fit = C[mask]

    if len(r_fit) < 3:
        return np.nan, np.nan, None

    logC = np.log(C_fit)

    # Linear fit: log C = intercept + slope * r
    slope, intercept = np.polyfit(r_fit, logC, 1)

    if slope >= 0:
        return np.nan, np.nan, None

    xi = -1.0 / slope

    # crude fit quality: RMS residual in log-space
    residuals = logC - (intercept + slope * r_fit)
    rms_resid = np.sqrt(np.mean(residuals**2))

    fit_info = {
        "r_fit": r_fit,
        "C_fit": C_fit,
        "slope": slope,
        "intercept": intercept,
```

```
        "rms_resid": rms_resid
    }

    return xi, rms_resid, fit_info
```

In [22]:

```
# ============================================================
# CORRELATION LENGTH SWEEP
# ============================================================

def correlation_length_sweep(
    g_values=np.linspace(0.5, 1.5, 11),
    N=48,
    M=48,
    delta_tau=0.25,
    n_therm=4000,
    n_measure=6000,
    measure_every=10,
    seed_base=12000,
    r_min=1,
    r_max=16
):
    """
    Estimate spatial correlation length xi(g).

    For each g:
      1. Run Monte Carlo.
      2. Save several correlation-function estimates.
      3. Average C(r).
      4. Fit exponential decay to estimate xi.
    """

    corr_results = {
        "g": [],
        "xi": [],
        "fit_error": [],
        "r_values": [],
        "C_values": [],
        "fit_info": []
    }

    for idx, g in enumerate(g_values):
        print(f"\nRunning correlation sweep: g = {g:.3f}")

        params = TFIMParams(
            N=N,
            M=M,
            g=float(g),
            J=1.0,
            delta_tau=delta_tau
        )

        rng = np.random.default_rng(seed_base + idx)
        K_s, K_tau = couplings(params)
        spins = initialize_lattice(N, M, ordered=True, rng=rng)

        # Thermalization
```

```
        for _ in range(n_therm):
            metropolis_sweep(spins, K_s, K_tau, rng)

        # Measurement
        C_samples = []

        for sweep in range(n_measure):
            metropolis_sweep(spins, K_s, K_tau, rng)

            if sweep % measure_every == 0:
                r_values, C_values = spatial_correlation(spins)
                C_samples.append(C_values)

        C_mean = np.mean(np.array(C_samples), axis=0)

        xi, fit_error, fit_info = estimate_correlation_length(
            r_values,
            C_mean,
            r_min=r_min,
            r_max=r_max
        )

        corr_results["g"].append(float(g))
        corr_results["xi"].append(xi)
        corr_results["fit_error"].append(fit_error)
        corr_results["r_values"].append(r_values)
        corr_results["C_values"].append(C_mean)
        corr_results["fit_info"].append(fit_info)

        print(
            f"g={g:.3f} | "
            f"xi={xi:.3f} | "
            f"fit RMS={fit_error:.3f}"
        )

    return corr_results
```

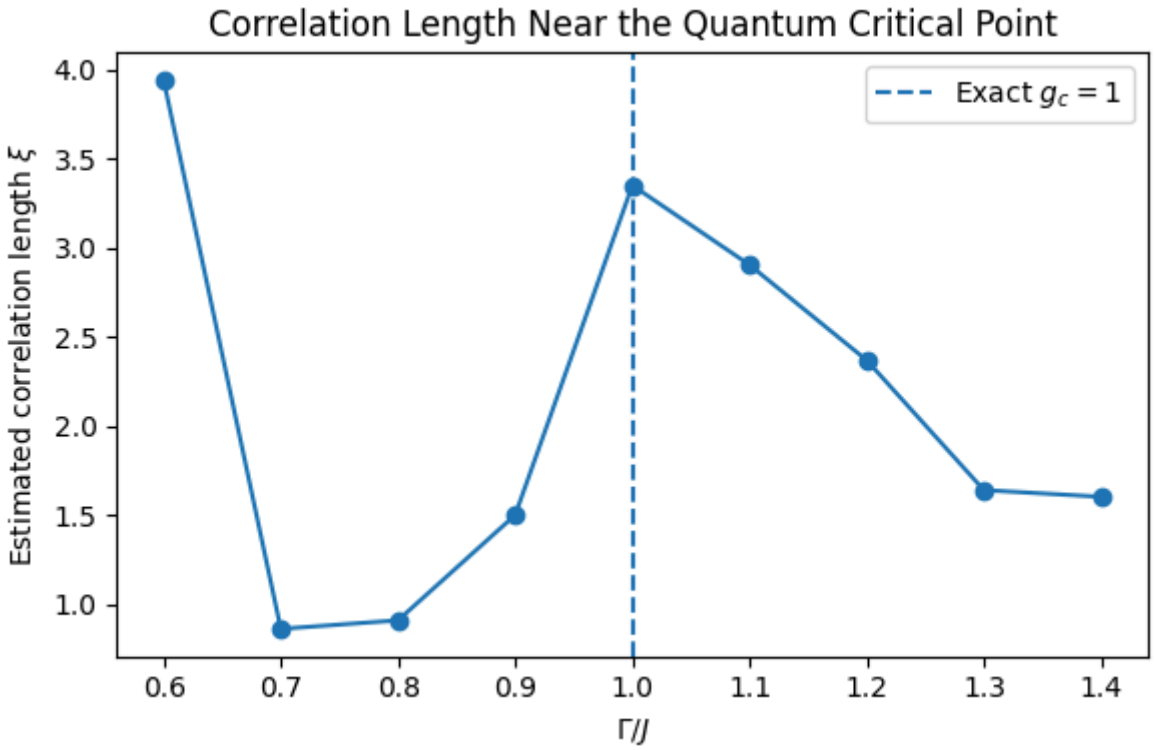
In [23]:

```
g_corr = np.linspace(0.6, 1.4, 9)

corr_results = correlation_length_sweep(
    g_values=g_corr,
    N=48,
    M=48,
    delta_tau=0.25,
    n_therm=3000,
    n_measure=5000,
    measure_every=10,
    seed_base=14000,
    r_min=1,
    r_max=14
)
```

```
Running correlation sweep: g = 0.600
g=0.600 | xi=3.942 | fit RMS=2.262

Running correlation sweep: g = 0.700
g=0.700 | xi=0.859 | fit RMS=0.074

Running correlation sweep: g = 0.800
g=0.800 | xi=0.907 | fit RMS=0.256

Running correlation sweep: g = 0.900
g=0.900 | xi=1.499 | fit RMS=0.058

Running correlation sweep: g = 1.000
g=1.000 | xi=3.351 | fit RMS=0.264

Running correlation sweep: g = 1.100
g=1.100 | xi=2.905 | fit RMS=0.203

Running correlation sweep: g = 1.200
g=1.200 | xi=2.368 | fit RMS=0.234

Running correlation sweep: g = 1.300
g=1.300 | xi=1.639 | fit RMS=0.357

Running correlation sweep: g = 1.400
g=1.400 | xi=1.601 | fit RMS=0.158
```

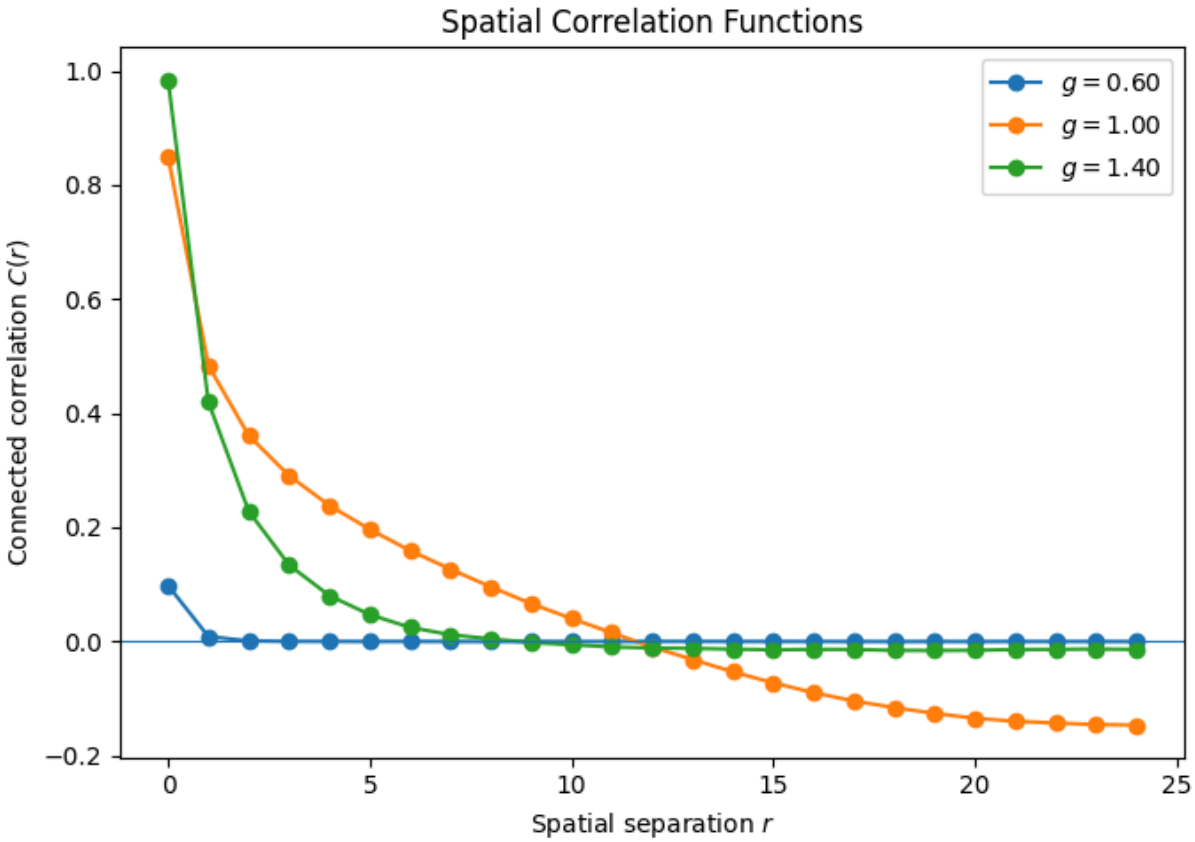
In [24]:

```python
# ============================================================
# CORRELATION LENGTH VS GAMMA/J
# ============================================================

plt.figure(figsize=(6, 4))

plt.plot(
    corr_results["g"],
    corr_results["xi"],
    marker="o"
)

plt.axvline(1.0, linestyle="--", label=r"Exact $g_c=1$")

plt.xlabel(r"$\Gamma/J$")
plt.ylabel(r"Estimated correlation length $\xi$")
plt.title("Correlation Length Near the Quantum Critical Point")
plt.legend()
plt.tight_layout()
plt.show()
```



In [25]:

```python
# ============================================================
# REPRESENTATIVE CORRELATION FUNCTIONS
# ============================================================

plt.figure(figsize=(7, 5))

for target_g in [0.6, 1.0, 1.4]:
    idx = np.argmin(np.abs(np.array(corr_results["g"]) - target_g))

    r = corr_results["r_values"][idx]
    C = corr_results["C_values"][idx]

    plt.plot(
        r,
        C,
        marker="o",
        label=rf"$g={corr_results['g'][idx]:.2f}$"
    )

plt.axhline(0, linewidth=0.8)
plt.xlabel(r"Spatial separation $r$")
plt.ylabel(r"Connected correlation $C(r)$")
plt.title("Spatial Correlation Functions")
plt.legend()
plt.tight_layout()
plt.show()
```


Spatial Correlation Functions
Connected correlation $C(r)$
Spatial separation r
$g = 0.60$
$g = 1.00$
$g = 1.40$
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0
5
10
15
20
25

In [ ]: