

Aging of ring polymeric topological glass formers via thermal quench

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(Received 30 April 2025; accepted 25 April 2026; published 6 July 2026)

We investigate the nonequilibrium glassy dynamics of dense, topologically constrained ring-polymer systems subjected to instantaneous thermal quenches, using large-scale molecular dynamics simulations. We show that the onset of dynamical arrest is strongly controlled by polymer stiffness, with increasing rigidity enhancing configurational constraints and shifting the estimated glass transition temperature to higher values. Below this threshold temperature, the system exhibits clear aging behavior, manifested through the waiting-time dependence of two-time correlation functions, with the corresponding structural relaxation approximately displaying a simple aging scenario. A key feature of these systems is the emergence of long-lived threaded rings, upon quenching, which act as persistent topological constraints, and the threading relaxation is shown to be correlated with aging dynamics. At the collective level, persistent threading leads to pronounced spatial heterogeneity, manifested as clustering of centers of mass of the rings. Cluster formation is maximized near the glass transition and is enhanced by polymer stiffness, while aging primarily affects the kinetics of cluster participation rather than their characteristic size. Overall, our study establishes a direct connection between polymer stiffness, topological constraints, spatial heterogeneity, and aging dynamics in ring-polymer glasses.

DOI: [10.1103/tdfs-l7fw](https://doi.org/10.1103/tdfs-l7fw)

I. INTRODUCTION

Glass-forming liquids transform into a glassy state when rapidly quenched to low temperatures [1]. Empirically, the glass transition temperature is defined as the temperature at which the material becomes exceedingly viscous, typically around 10^{12} poise [2]. Below this transition temperature, the material struggles to reach equilibrium within accessible observation timescales, and its properties continue to evolve even when held at a constant temperature—this phenomenon is known as aging [3–6]. Such out-of-equilibrium behavior arises from the complex underlying energy landscape of glass-forming materials, where the system becomes trapped in local minima, resulting in extremely slow relaxation dynamics [3,7]. Aging behavior has been observed across a wide range of glassy materials—including colloidal glasses, polymers, and metallic glasses—where structural and dynamical properties exhibit slow temporal evolution [8–14]. Understanding aging therefore remains a central question in exploring the slow dynamics and long-term stability of these materials.

Ring-polymer systems with tunable stiffness provide a versatile model for investigating glass formation and aging in soft, deformable particlelike systems, where internal degrees of freedom play a central role, in contrast to conventional colloids [15–18]. Owing to their closed-loop architecture, ring polymers exhibit rheological behavior distinct from that of linear chains. Several studies have demonstrated that ring polymers display unconventional stress-relaxation dynamics, primarily due to the absence of free ends. This prevents reptationlike motion and instead creates entanglement constraints mediated by threading effects [19–29]. These topological constraints induce dynamical slowdowns analogous to crowding effects in dense colloidal suspensions, making ring polymers valuable model systems for exploring glassy dynamics. By tuning backbone stiffness, one can systematically modulate their phase behavior—akin to tuning softness or interaction strength in colloidal assemblies to control proximity to the glass transition [30–34].

Despite these parallels, the aging dynamics of topologically constrained ring polymers remain underexplored. While studies on linear polymers have shown that chain stiffness and density significantly influence the glass transition temperature [11,35–37], ring polymers introduce an additional layer of complexity through threading interactions. Unlike conventional colloidal or polymeric glasses, where relaxation is governed by caging or linear-chain entanglements, ring polymers experience unique topological frustrations arising from threading-mediated constraints that hinder structural relaxation and reorganization [38–43]. Previous work has indicated that stiffness modulates the dynamical slowdown in mixed-stiffness ring-polymer systems [43,44]; however, a systematic characterization of aging dynamics as a function of stiffness

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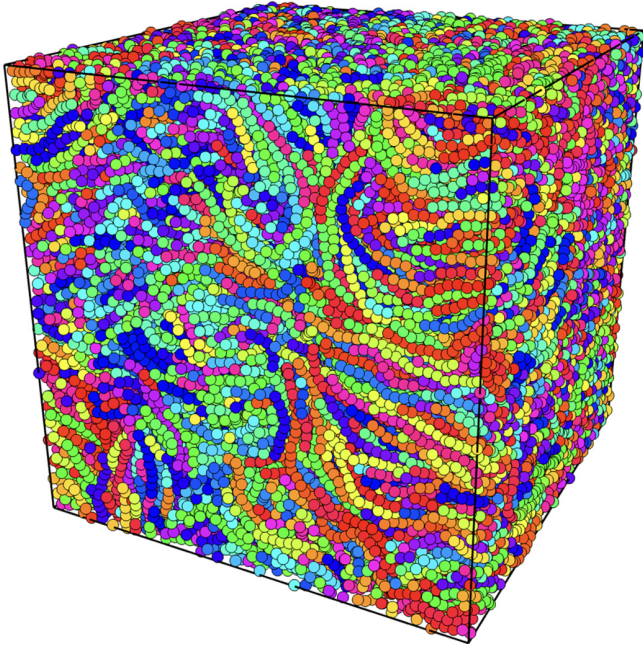


FIG. 1. A representative snapshot of the initial configuration of the system. The system consists of 1000 nonconcatenated ring polymers with 100 monomers per each polymer.

is still lacking. Investigating how polymer stiffness affects threading dynamics and determining the glass transition temperature in ring polymer melts can thus provide crucial insight into how topological constraints govern aging and structural relaxation, deepening our understanding of glass formation in these unique polymeric systems.

II. METHODS

We employ molecular dynamics simulations to investigate the aging behavior of dense melts composed of $N = 1000$ nonconcatenated ring polymers, each containing 100 monomers. We work at a monomer number density of $\rho \approx 0.56$. A representative equilibrated configuration is shown in Fig. 1. The initial state is generated by randomly packing the polymers, followed by equilibration in the canonical (constant number of particles N , volume V , and temperature T) ensemble (NVT) ensemble at a high temperature of $T = 15$ using a Nosé-Hoover thermostat. After equilibration, we do an additional run of $t = 10^5$ using a time step of $\delta t = 0.001$ to ensure thermalization in the high-temperature state. This protocol is the same for all the four ring-polymer stiffness values investigated in this work. The equilibrated configurations are then instantaneously quenched to low temperatures, and the dynamics are followed for a time window of $t = 1.5 \times 10^6$, using a time step of $\delta t = 0.005$.

Model

In our system, the monomers in a polymer interact via the finitely extensible nonlinear elastic (FENE) potential,

$$U_{\text{FENE}}(d_{ij}) = \begin{cases} -0.5\kappa R_0^2 \ln[1 - (\frac{d_{ij}}{R_0})], & d_{ij} < R_0, \\ \infty, & d_{ij} \geq R_0. \end{cases} \quad (1)$$

Here, d_{ij} denotes the distance between two bonded monomers, which must be smaller than $R_0 = 1.5$, the cutoff for the maximum allowable bond length, and $\kappa = 30$ represents the strength of the FENE potential. The FENE potential ensures that polymers cannot be stretched indefinitely. The elasticity of the polymers is modeled using the Kratky-Porod model [40], given by

$$U_{\text{angle}}(\theta_i) = K_\theta [1 - \cos(\theta_i - \pi)]. \quad (2)$$

where, K_θ represents the stiffness of the polymer and θ_i is the angle formed at the i th monomer site. In this study, we investigate four distinct stiffness values: $K_\theta = 1, 5, 10, 20$, where $K_\theta = 1$ corresponds to flexible polymers, $1 < K_\theta \leq 10$ to semiflexible polymers, and $K_\theta > 10$ to rigid polymers. Each simulated system is monodisperse, meaning that all polymers within a given system share the same stiffness value. Nonbonded monomer pairs interact via the Lennard-Jones potential,

$$U_{\text{pair}}(r_{ij}) = \begin{cases} 4\varepsilon [(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^6 + \frac{1}{4}], & r_{ij} \leq 2^{\frac{1}{6}}\sigma, \\ 0, & r_{ij} > 2^{\frac{1}{6}}\sigma, \end{cases} \quad (3)$$

where $\sigma = 1$ is the monomer diameter and ε is the energy scale. For simplicity, we set $\varepsilon = 1$ for our simulations. We truncate the potential so that only repulsive interactions occur at short distances.

III. RESULTS

A. Identification of thermal glassy regime

We first identify the regime within the phase space of ring stiffness and ambient temperature where the system exhibits glassy dynamics. For each stiffness value (K_θ), the system is quenched from a high-temperature equilibrium state to several lower target temperatures (T). By monitoring the potential energy (E_{pot} , Figs. 14 and 15) over a specified time window following the quench, we ascertain whether the system reaches equilibrium or remains out of equilibrium at these target temperatures [45–48].

To obtain a quantitative estimate of the temperature range over which ring-polymer systems of varying stiffness display glassy behavior, we examine their dynamical properties. Specifically, we identify the temperature at which diffusive dynamics cease, marking the onset of nonergodic behavior and defining the regime appropriate for probing aging phenomena. For this purpose, we compute the mean-square displacement (MSD) of the ring-polymer center of mass [22],

$$\langle g_3(t) \rangle = \frac{1}{N} \sum_{k=1}^N [\bar{R}_{\text{cm}}^k(t) - \bar{R}_{\text{cm}}^k(0)]^2, \quad (4)$$

where $\bar{R}_{\text{cm}}^k$ denotes the center-of-mass coordinates of the k th ring.

Figure 2 displays the MSD at different temperatures for two contrasting stiffness values, $K_\theta = 1$ and 20, highlighting the thermal range where asymptotic diffusion [$g_3(t) \sim t$] is observed; results for intermediate stiffnesses are shown in Appendix B (see Fig. 16). To quantify the extent of diffusion, we extract the diffusion coefficient (D) from these MSD curves and plot its temperature dependence in Fig. 2(c). As

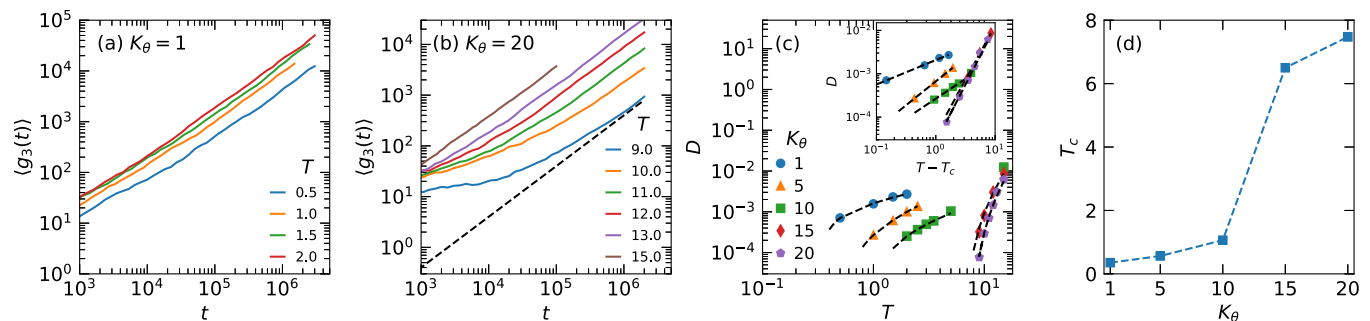


FIG. 2. (a), (b) Mean-square displacement of the center of mass of polymers, $g_3(t)$, for $K_\theta = 1, 20$, where t is the time since thermal quench. (c) Diffusion coefficient D as a function of temperature; the dashed lines correspond to power-law fits $\sim (T - T_c)^\gamma$. Inset: D plotted as a function of $T - T_c$ for all stiffness values. (d) Estimated T_c for dynamical arrest as a function of polymer stiffness K_θ ; the dotted line is a guide to the eye.

expected, D decreases systematically as temperature decreases for all stiffness values. At a fixed temperature (e.g., $T = 2$), the diffusion coefficient of flexible polymers exceeds that of stiffer polymers, underscoring the pronounced dependence of diffusion on K_θ . The diffusion data clearly indicate that dynamical arrest ($D \rightarrow 0$) occurs at progressively higher temperatures with increasing stiffness.

To estimate the temperature of dynamical arrest (T_c) more quantitatively, we perform power-law fits of the form $D \sim (T - T_c)^\gamma$ [dashed lines in Fig. 2(c)]. Fits were performed over the final decade of accessible diffusive data, where the power-law dependence was most robust, as confirmed by the log-log representation of D versus $T - T_c$ shown in the inset of Fig. 2(c). The resulting T_c values are plotted in Fig. 2(d). The loss of long-time diffusion, and hence of equilibrium, is found at $T_c \approx 0.35, 0.56, 1.06, 6.50$, and 7.47 (rounded to two decimal places) for polymer stiffnesses $K_\theta = 1, 5, 10, 15$, and 20 , respectively. These temperatures serve as reference scales analogous to the mode-coupling temperature, where the diffusion coefficient theoretically vanishes in a power-law manner. The exponent γ shows a slight stiffness dependence, implying that increasing K_θ alters the underlying relaxation pathways. The collapse of the diffusion data when plotted as a function of $T - T_c$ [inset of Fig. 2(c)] further confirms the validity of the power-law scaling, while the variation in the exponent γ suggests a stiffness-dependent change in fragility—an aspect warranting further study. The observed increase in T_c with stiffening confirms that rigid polymers enter the glassy regime at higher temperatures, reflecting enhanced configurational constraints. In ring-polymer melts, topological effects, particularly threading interactions, impose additional constraints beyond those of conventional entanglement, elevating T_c beyond values expected from chain entanglement alone [11,35,36].

Having estimated the thermal regimes for which diffusive translational motion of the rings is expected to be observed, we now delve into probing for aging behavior at lower temperatures, which we discuss in the next section.

B. Aging dynamics

In equilibrated systems, temporal correlation functions depend solely on the time difference between measurements, reflecting time-translational invariance. However, in glassy

systems, equilibration becomes increasingly difficult within accessible simulation or experimental timescales as the ambient temperature approaches and drops below the characteristic temperature (T_c). This occurs because relaxation times grow rapidly with decreasing temperature, causing the system to fall progressively out of equilibrium. Consequently, correlation functions depend not only on the time difference but also explicitly on the initial measurement time, known as the waiting time (t_w), making them two-time quantities [47]. This t_w dependence is a hallmark of aging behavior.

To explore aging dynamics in our system, we analyze the waiting-time-dependent mean-square displacement of the polymer center of mass (COM) and the self-intermediate scattering function (ISF). We investigate how polymer stiffness (K_θ) and temperature (T) influence dynamical slowdown, subdiffusive behavior, and aging phenomena, thereby elucidating distinctive features of aging in ring-polymer systems compared to conventional polymer and colloidal glasses. Figures 3(a)–3(d) present the waiting-time-dependent MSD for ring polymers following instantaneous quenches from a high-initial temperature to target temperatures below their respective T_c values, as indicated in each subplot for each stiffness K_θ . We observe that at intermediate to longer timescales, the MSD curves consistently display subdiffusive behavior and pronounced dependence on waiting time. This dependence strengthens at larger t_w , reflecting a gradual dynamical slowdown as the system ages. Aging signatures appear clearly as plateaus in $g_3(t_w, \Delta t)$ at larger waiting times, indicative of particle-caging effects arising from neighboring rings. These characteristics observed in ring-polymer MSDs qualitatively mirror other soft-glassy systems, such as colloidal hard spheres [48]. Further, we analyze the aging dynamics of the monomers with respect to the center-of-mass of the rings; the measured $g_2(t_w, \Delta t)$ is shown in Figs. 3(e) and 3(f) for the largest and smallest ring stiffness that we have studied, viz., $K_\theta = 1, 20$. Note that because of the ring constraint, g_2 is always bounded by the effective size of the ring at any temperature; however, it provides information about the transient internal conformational relaxation [22]. We observe that not only the transient dynamics is age dependent, but the asymptotic bound is also weakly age dependent: the longer the waiting time, the larger the plateau height. Meanwhile, the age-dependent transient relaxation, which is observed to be more sluggish for larger t_w , also has dependence on ring

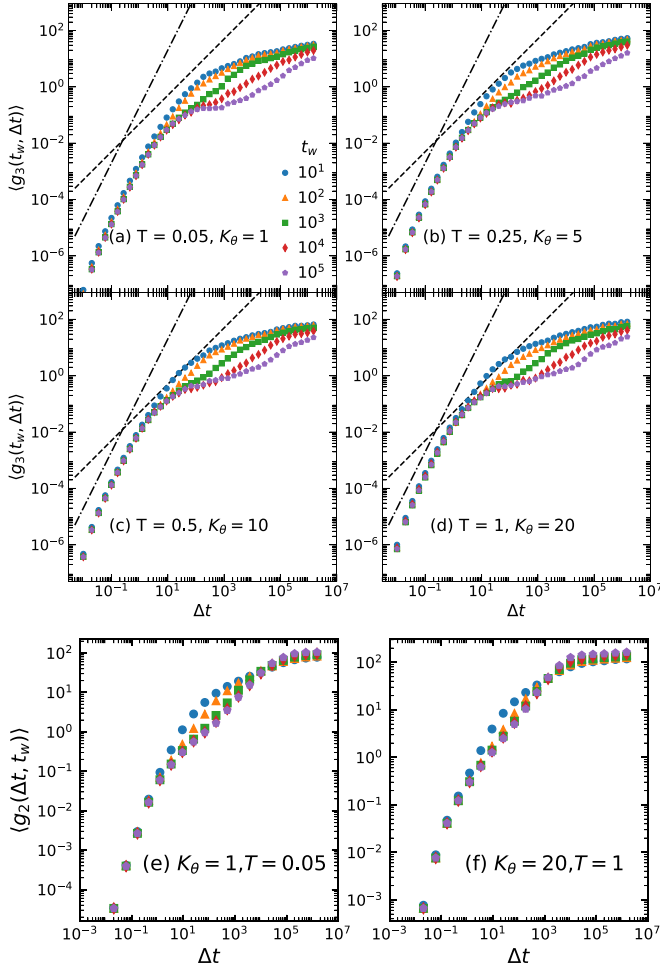


FIG. 3. (a)–(d) Mean-square displacement of the center of mass of polymers, $g_3(t_w, \Delta t)$, as a function of waiting time (t_w) for different stiffness values and temperatures, as marked. (e), (f) Waiting-time dependence of the mean-square displacement of the monomers with respect to the center of mass of the chain, $g_2(t_w, \Delta t)$, for two different stiffness values.

stiffness, with the variations more visible for $K_\theta = 1$ due to greater flexibility. Overall, the g_3 and g_2 measurements reflect the consequences of unique topology of ring polymers, which imposes additional constraints that strongly influence their aging dynamics, as discussed in more details later.

The age-dependent self-intermediate scattering function, $F_s(q, t_w, t)$, quantifies temporal correlations of density fluctuations and is widely used to characterize relaxation dynamics in glass-forming liquids. It is defined as

$$F_s(q, t_w, t) = \frac{1}{N} \sum_{k=1}^N e^{i\vec{q} \cdot [\vec{R}_{\text{cm}}^k(t+t_w) - \vec{R}_{\text{cm}}^k(t_w)]}, \quad (5)$$

where the summation is over all ring polymers and $\vec{R}_{\text{cm}}^k$ denotes the center-of-mass coordinates of the k th ring polymer. Unlike the simple exponential decay observed in liquids, supercooled systems display slow, nonexponential decay of the ISF. This results from activated hopping between multiple minima in a rugged potential-energy landscape, which

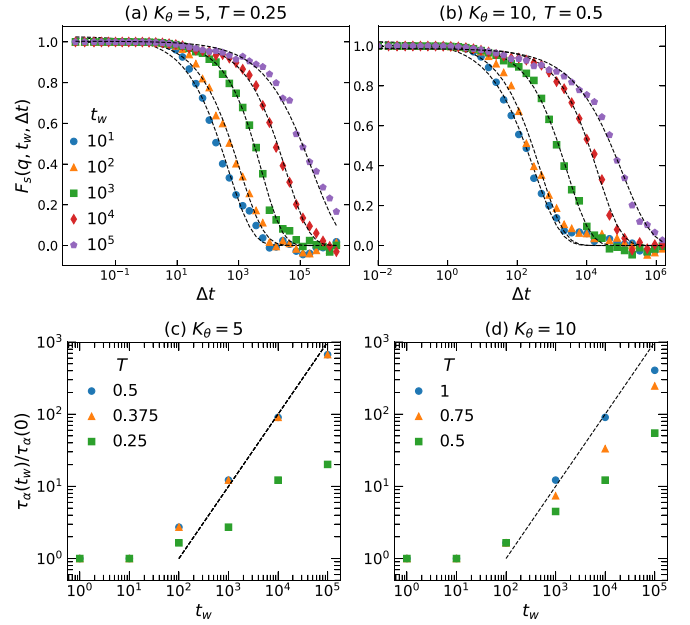


FIG. 4. (a), (b) Waiting-time dependence of the self-intermediate scattering function, $F_s(q, t_w, \Delta t)$, for $K_\theta = 5$ and 10, respectively, computed at $q = 1$. The dashed lines indicate stretched-exponential fits. (c), (d) Relaxation time τ_α as a function of waiting time t_w for $K_\theta = 5$ and 10, respectively, at different temperatures below the transition temperature ($T < T_c$), with timescales rescaled by $\tau_\alpha(0)$.

becomes increasingly prominent as the glass transition is approached [46,47].

Like the MSD discussed above, the ISF also exhibits aging behavior, as shown in Figs. 4(a) and 4(b) for $q = 1$, corresponding to a length scale, which is approximately close to typical values of the radius of gyration. To compare the results for $K_\theta = 1, 20$ (see Fig. 19). At long timescales, the ISF decays increasingly slowly with larger t_w , indicating progressive slowdown in structural relaxation as the system ages. The data can be reasonably described by stretched-exponential fits. For each dataset, the fit quality was evaluated over two decades of Δt , yielding stretching exponents $\beta \simeq 0.35$ – 0.5 , consistent with typical glass-forming systems. The aging-dependent relaxation is quantified via the relaxation time $\tau_\alpha(t_w)$, defined as the time at which $F_s(q, t_w, \tau_\alpha) = 1/e$. Figures 4(c) and 4(d) show the waiting-time dependence of τ_α for $K_\theta = 5$ and 10 at different temperatures. For reference, the dashed lines correspond to a simple aging scenario, $\tau_\alpha \sim t_w$. For small waiting times, τ_α remains nearly constant, consistent with transient relaxation dominated by initial high-temperature effects (as also seen in the MSD data, Fig. 3). For $t_w > 10^2$, τ_α increases significantly with age, and flexible polymers display a more pronounced rise compared to the rigid systems ($K_\theta = 10$), underscoring stiffness-enhanced dynamical constraints. For comparison, across all stiffness values, (see Fig. 20).

The observed waiting-time dependence of MSD and ISF is qualitatively consistent with studies of aging in colloidal and polymeric glasses [47,48]. However, the distinct topology and stiffness of ring polymers introduce additional constraints, leading to characteristic aging signatures, including sublinear growth of τ_α with t_w . Increased stiffness

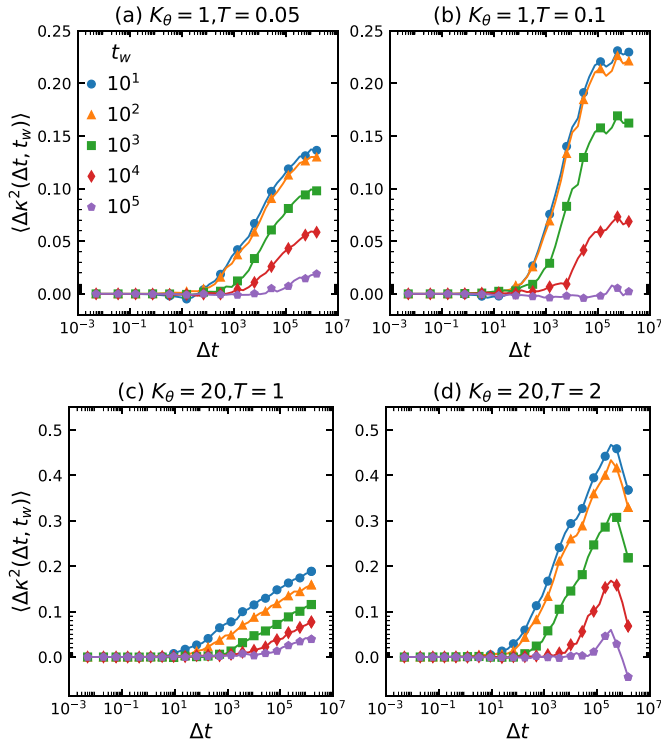


FIG. 5. Change in relative shape anisotropy $\langle \Delta \kappa^2(\Delta t, t_w) \rangle$ for different waiting times below the glass transition temperature. Upper panels correspond to flexible rings ($K_\theta = 1$) and lower panels to rigid rings ($K_\theta = 20$). The $\langle \cdot \rangle$ represent the average over all rings.

amplifies excluded-volume effects, restricting configurational rearrangements and intensifying aging. These findings align with observations in dense polymer melts, where stiffness delays relaxation and enhances dynamical heterogeneity [49]. The pronounced dependence of τ_α on both t_w and K_θ highlights the crucial roles of stiffness and waiting time in governing the aging dynamics of glassy ring-polymer systems. Moreover, the absence of free ends and the presence of threading impose unique topological constraints that further slow structural relaxation, clearly distinguishing their aging behavior from that of linear-polymer glasses. We examine these topological effects, particularly threading, in the next section.

C. Aging effects on ring conformations

Next, we analyze structural changes of polymers during aging. We focus on configurational observables such as the radius of gyration and the relative shape anisotropy. We ask how time evolution of changes in conformational measures depends on the waiting time t_w . We define the change in any observable s relative to the waiting time as

$$\Delta s(\Delta t, t_w) = s(t + t_w) - s(t_w). \quad (6)$$

This characterizes the aging effects in structural observables.

In Fig. 5, we show the change in relative shape anisotropy $\langle \Delta \kappa^2 \rangle$ [see Eq. (D1) for definition] for different waiting times, and we compare the results between the flexible (upper panel) and the more rigid polymer (lower panel) cases. The

measurements are done, for both K_θ values at two different temperatures, which are chosen slightly less than the respective T_c or further below, i.e., deeper into the glassy regime. In each of the cases, we observe that there is an increase in the shape anisotropy, i.e., $\langle \Delta \kappa^2 \rangle > 0$, with increasing observation time, and the onset of increase shifts systematically to the right as t_w increases. The crossover time at which $\langle \Delta \kappa^2 \rangle$ departs from zero increases monotonically with t_w . This is clear in Figs. 5(a) and 5(b), where each decade increase in t_w delays the onset of growth by a comparable factor in Δt . The increase in $\langle \Delta \kappa^2 \rangle$ indicates the transformation of rings from a nearly isotropic shape toward a disklike shape. At lower temperatures for each stiffness [Figs. 5(a) and 5(c)], the growth in $\langle \Delta \kappa^2 \rangle$ slows down as the system ages, which reflects the configurational arrest due to lack of thermal fluctuations. On the other hand, at temperatures closer to T_c [Figs. 5(b) and 5(d)], the behavior depends on the stiffness. For the rigid system ($K_\theta = 20$), we observe a sharp decline in $\langle \Delta \kappa^2 \rangle$ at long times, in contrast to the flexible system, which hints at a saturation in $\langle \Delta \kappa^2 \rangle$. Similar behavior is observed for other stiffness values as shown in Fig. 21. Stiffer systems undergo a significant relaxation process at temperatures close to the estimated T_c , whereas flexible systems do not exhibit such behavior. We note that the decline in $\langle \Delta \kappa^2 \rangle$ (also in $\langle \kappa^2 \rangle$, see Fig. 18) at long times indicates a structural relaxation of ring polymers from a doubly folded linear configuration to an extended and open structure. We will discuss later the ramifications for such shape changes.

We observe a similar aging dependency of $\langle \Delta R_g \rangle$ in Fig. 6. All the curves show a time lag in growth, with sluggish growth at lower temperatures compared to the higher temperatures [Figs. 6(a)–6(d)]. The growth in $\langle \Delta R_g \rangle$ slows down as the system ages for all the stiffness values. However, in contrast to $\langle \Delta \kappa^2 \rangle$, $\langle \Delta R_g \rangle$ does not decline at long times, even at higher temperatures below T_c . The increase in radius of gyration accompanied by a decrease in relative shape anisotropy suggests a swelling of rings to a disklike shape. Results for other stiffness values at their respective glass temperatures are provided in Fig. 22.

D. Threading analysis

Ring polymers, unlike linear polymers, are topologically constrained, making structural rearrangements difficult, particularly at low temperatures. The absence of free ends prevents ring polymers from undergoing reptation—the primary relaxation mechanism in linear-polymer melts. Instead, their unique topology allows for *threading*, a phenomenon in which one ring polymer passes through the contour of another, introducing additional entanglement constraints [43]. Formally, threading is defined by the intersection of bond vectors (monomer-monomer bonds) of one ring polymer with the triangular planes forming the minimal surface of another ring polymer (see Fig. 7). Specifically, if the bond vectors of ring A intersect with the minimal surface of ring B, ring A is said to thread into ring B. To quantify threading, we define N_{th} as the number of bonds of ring A located between two successive intersections. To simplify calculations, we divide each ring into an odd side and an even side and count the bonds on the odd side (N_{th}^{odd}). Given the absence of free ends, the total

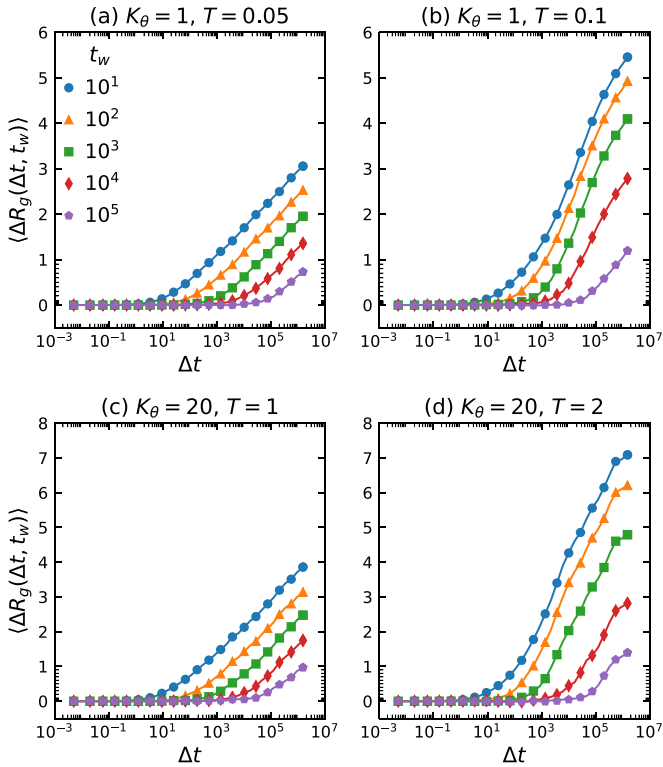


FIG. 6. Change in radius of gyration $\langle \Delta R_g(\Delta t, t_w) \rangle$ for different waiting times. Results are shown for flexible and rigid systems at temperatures close to their respective glass temperatures. The $\langle \cdot \rangle$ represent the average over all rings.

number of bonds satisfies the relation $N_{th}^{odd} + N_{th}^{even} = N_{ring}$, where N_{ring} is the total number of bonds in a ring. Finally, we define the degree of threading as

$$\Delta(t) = 1 - \left| \frac{2 \sum_{i=odd} N_{th}^i}{N_{ring}} - 1 \right|. \quad (7)$$

Equation (7) provides a quantitative measure of threading events in the system. A value of $\Delta(t) = 0$ corresponds to no threading, i.e., when $\sum_{i=odd} N_{th}^i = 0$, whereas a maximum value of $\Delta(t) = 1$ occurs when a ring is perfectly bisected by

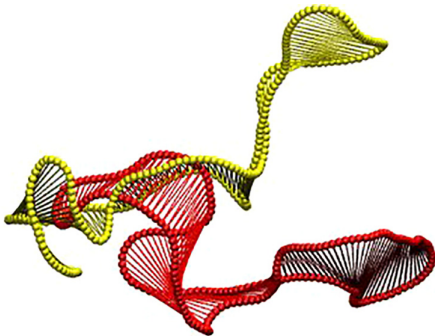


FIG. 7. Schematic representation of two threaded polymers with triangulated surface. The figure is taken from Ref. [43] with permission.

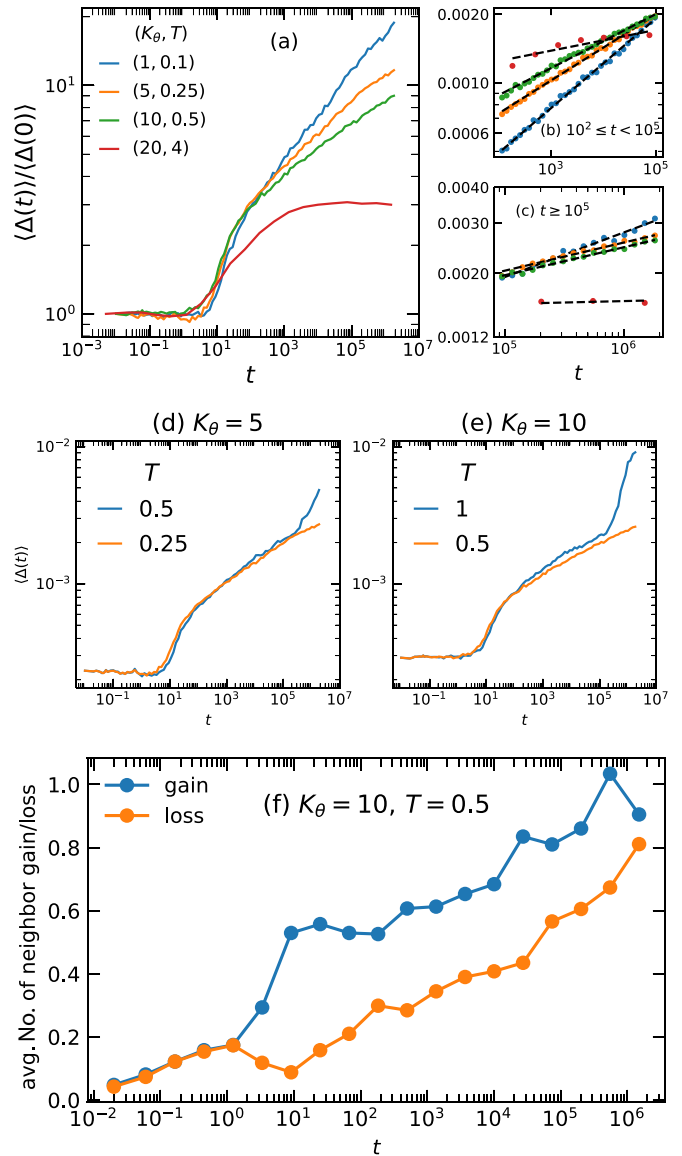


FIG. 8. (a) Time evolution of the degree of threading relative to initial state, $\Delta(t)/\Delta(0)$, for various stiffness values $K_\theta = 1, 5, 10, 20$ at their respective glassy state points discussed in Figs. 4(d) and 4(e). Time evolution of $\Delta(t)$ at two different temperatures, for $K_\theta = 5, 10$, respectively. (f) Number of threading neighbor gain/loss events over time, measured at the state point $K_\theta = 10, T = 0.5$.

another, such that $\sum_{i=odd} N_{th}^i = N_{ring}/2$. Applying Eq. (7), we compute the degree of threading for each ring polymer and obtain an average over all rings to quantify the system-wide degree of threading over time.

We first analyze how the extent of threading evolves as the system is quenched from a high-temperature liquid state into a low-temperature topological glassy state. Since a topological glass is characterized by a high degree of threading, it is expected that the initially equilibrated high-temperature liquid will exhibit significantly lower threading. This is indeed observed in Fig. 8(a), which shows the time evolution of the average degree of threading $\Delta(t)$ for ring polymers with stiffness values $K_\theta = 1, 5, 10, 20$ following a quench to temperatures below their respective T_c . At short times

($t < 10$), threading remains nearly constant across all stiffnesses, consistent with the persistence of high-temperature initial conditions and the dominance of local fluctuations. For $K_\theta = 1, 5$, and 10 , threading increases gradually and with similar overall trends. Despite differences in stiffness, these systems retain sufficient conformational flexibility and configurational freedom for threading to develop progressively over time, without severe hindrance. In contrast, the $K_\theta = 20$ system exhibits markedly different behavior. While initial growth is visible, threading saturates rapidly and remains flat at long timescales, indicating strong dynamical arrest. The high stiffness in this regime imposes significant steric and topological constraints, suppressing large-scale rearrangements required for further interpenetration. This stagnation in $\Delta(t)$ growth reflects a glassy state dominated by persistent threadings and limited mobility.

To further quantify long-time threading dynamics, data for $t \geq 10^5$ were fitted to a power-law relationship, $\Delta(t) \sim t^\eta$. Figure 8(b) shows the fits at early times, with the exponent η capturing the stiffness dependence of long-time threading behavior. The extracted η values range from 0.04 to 0.2, highlighting the distinct dynamic regimes introduced by polymer stiffness. Figure 8(c) shows fits at later times, where all stiffness values except $K_\theta = 20$ exhibit similar trends, indicating that the highest stiffness value behaves distinctly. Fits were performed over the last decade of well-converged data, with uncertainties in η within ± 0.02 .

In Figs. 8(d) and 8(e), we analyze how temperature affects threading growth for polymers with stiffness $K_\theta = 5$ and 10 by comparing dynamics at two temperatures: one significantly below T_c and another near T_c . Initially, threading growth is similar at both temperatures; however, at later times, distinct deviations emerge. At higher temperatures near T_c , threading growth shows a secondary rapid increase at long times, suggesting that enhanced thermal fluctuations facilitate additional structural rearrangements and new threading events—a mechanism suppressed deep in the glassy regime.

Figure 8(f) provides microscopic insight by tracking the number of gain and loss events associated with threading over time, specifically for polymers with $K_\theta = 10$ quenched to a glassy state at $T = 0.5$. The gain curve increases more steeply than the loss curve, indicating that new threading events continue to form during the system's evolution and, once established, are not easily undone. At short times ($t < 10$), both gain and loss rates remain low, consistent with limited large-scale rearrangements. With increasing time, the rate of threading events accelerates, signaling the onset of structural reorganization. However, threading-loss events remain comparatively infrequent, underscoring the persistent nature of topological constraints formed during aging. The sustained increase in threading reinforces the notion that ring polymers experience durable topological constraints, particularly at low temperatures, leading to significantly slowed dynamics and characteristic glassy rigidity.

To quantify aging effects on threading dynamics, we calculate the average threading duration between pairs of rings. We define the threading matrix $P_{ij}(t)$ at time t as

$$P_{ij}(t) = \begin{cases} 1, & \text{if the } i\text{th ring is threaded to the } j\text{th,} \\ 0, & \text{otherwise.} \end{cases} \quad (8)$$

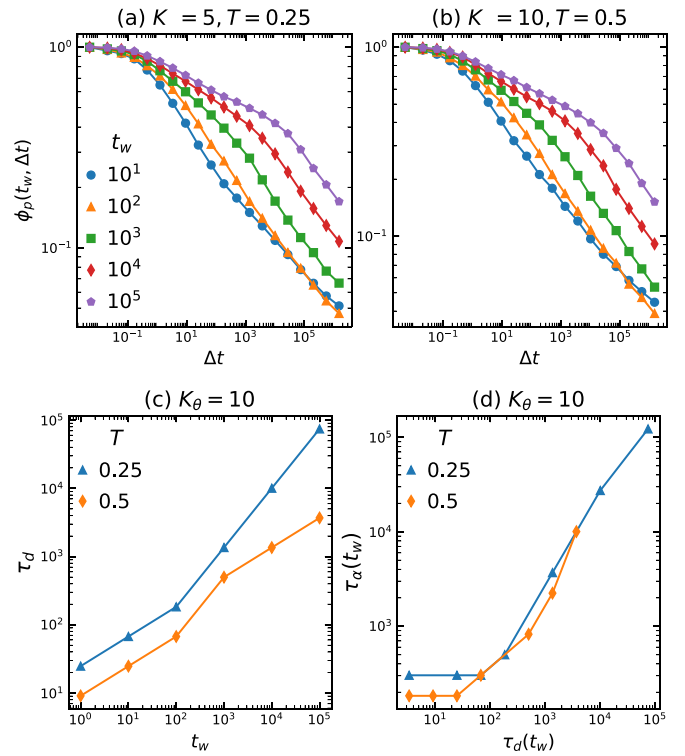


FIG. 9. Age dependence of the correlation function $\phi_p(t_w, \Delta t)$ measured at the state points: (a) $K_\theta = 5$, $T = 0.25$ and (b) $K_\theta = 10$, $T = 0.5$. (c) Variation of the characteristic discontinuity time, τ_d , extracted from $\phi_p(t_w, \Delta t)$, with age t_w , shown for $K_\theta = 10$, at temperatures of $T = 0.5, 1.0$. (d) Correlation of structural relaxation time, τ_α , with threading discontinuity time, τ_d , as obtained via their respective age dependence and computed for the state points shown in panel (c).

Here, $P_{ii} = 0$, i.e., self-threading events are excluded. Also, when the i th polymer is threaded to the j th, $P_{ij} = 1$, but the converse is not necessarily true, i.e., $P_{ji} \neq 1$. At any point in time, $P_{ij}(t)$ is an $N \times N$ matrix, where N is the number of polymers. Using this matrix, we define the correlation function [50] as

$$\phi_p(t_w, t) = \left\langle \frac{1}{N} \sum_{j=1}^N P_{ij}(t + t_w) P_{ij}(t + t_w - \delta t) \cdots P_{ij}(t_w) \right\rangle, \quad (9)$$

where $\langle \cdots \rangle$ denotes an average over all rings. When two rings unthread, $P_{ij}(t)$ changes from $1 \rightarrow 0$; therefore, the correlation function $\phi_p(t_w, t)$ tracks such unthreading events as a function of waiting time t_w , thereby measuring threading persistence.

Figures 9(a) and 9(b) show the waiting-time dependence of $\phi_p(t_w, t)$ for ring polymers with stiffness values $K_\theta = 5$ and 10 ; data for other stiffnesses are provided in Appendix G. At short times ($t < 10$), $\phi_p(t_w, t) \approx 1$ across all waiting times, reflecting the ballistic regime where monomers remain highly correlated with their initial positions. The initial sharp drop at small t_w arises from transient effects following the high-temperature quench. As time progresses, the decay of $\phi_p(t_w, t)$ slows markedly for larger t_w , demonstrating progressive dynamical slowdown characteristic of aging in glassy

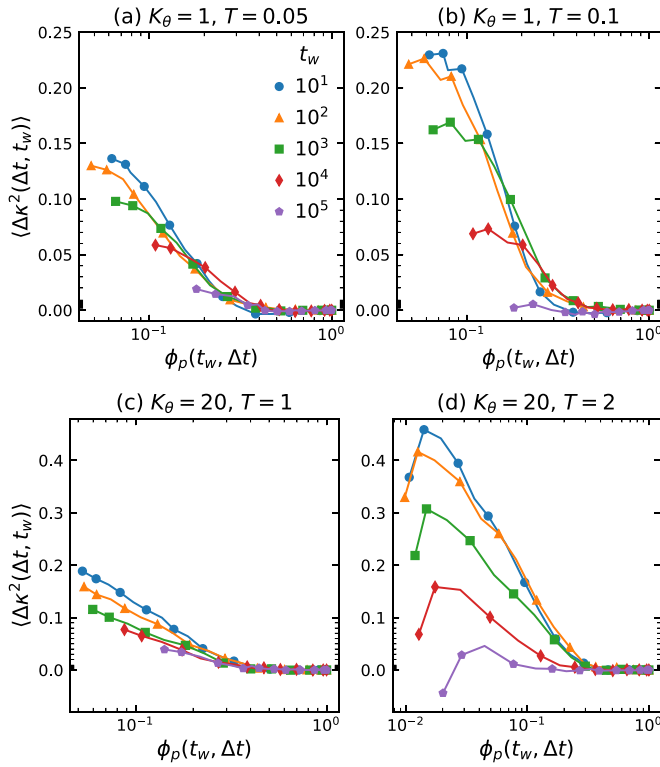


FIG. 10. Correlation between shape relaxation and threading persistence for flexible and stiff ring polymers. The mean-squared change in shape anisotropy, $\langle \Delta k^2(\Delta t, t_w) \rangle$, is plotted as a function of the threading persistence function $\phi_p(t_w, \Delta t)$ for different waiting times t_w . Panels (a) and (b) correspond to flexible rings ($K_\theta = 1$) at temperatures $T = 0.05$ and $T = 0.1$, respectively, while panels (c) and (d) show stiff rings ($K_\theta = 20$) at $T = 1$ and $T = 2$, respectively.

systems. Thus, threading decorrelation effectively captures signatures of aging dynamics.

We quantify this decorrelation using the characteristic discontinuity timescale τ_d , defined as the time at which $\phi_p(\tau_d) = 0.3$, corresponding to 70% decorrelation of initially threaded rings. Figure 9(c) shows that τ_d increases systematically with waiting time t_w , indicating that unthreading becomes progressively slower as the system ages. Thermal effects are also evident: At higher temperatures, τ_d is smaller and unthreading faster, suggesting that reduced thermal fluctuations amplify the role of topological constraints in glassy dynamics. Stretched exponential fits to $\phi_p(t_w, t)$ yield stretching exponents $\beta_p \simeq 0.2\text{--}0.4$, consistent with the slow decorrelation typical of topologically constrained systems (see Figs. 23 and 24). We now probe the relationship between relaxation of topological constraints and conformational changes, by correlating threading persistence with shape fluctuations. In Fig. 10, we plot the mean-squared change in the shape anisotropy, $\langle \Delta k^2(\Delta t, t_w) \rangle$, as a function of the threading persistence function $\phi_p(t_w, \Delta t)$ for different waiting times t_w . The top panels (a) and (b) correspond to flexible rings ($K_\theta = 1$), while the bottom panels (c) and (d) show the same analysis for stiff rings ($K_\theta = 20$), at the temperatures as marked. In all cases, we note that threading decorrelation is related to significant change in relative shape anisotropy, i.e., Δk^2 starts to increase when ϕ_p tends to fall below 0.4.

For flexible rings [Figs. 10(a) and 10(b)], we observe that the data collapses across waiting times, at both the temperatures analyzed. However, for higher temperatures, there is a larger change in Δk^2 as noted earlier. This suggests that shape relaxation in flexible rings is primarily governed by thermal fluctuations when the initial topological constraints change.

In contrast, stiff rings display a different behavior [Figs. 10(c) and 10(d)]. The data for the different t_w do not collapse together like what is observed for the flexible rings. Further at the temperature near T_c , $\langle \Delta k^2 \rangle$ exhibits pronounced, nonmonotonic behavior as a function of ϕ_p . Moreover, as the waiting time increases, the onset of shape relaxation is pushed to progressively lower values of ϕ_p , demonstrating that upon aging, shape changes occur later than when the initial threaded network decorrelates.

This analysis shows that polymer stiffness determines the coupling between shape relaxation and threading persistence, while temperature governs the accessibility of this coupling. This coupling between topology and conformational relaxation indicates possible spatial organisation of the interconnected rings, which we explore next through an analysis of cluster formation and its temporal evolution.

E. Cluster dynamics

The threading analysis above establishes that dynamical arrest in ring-polymer melts is governed by long-lived, stiffness-dependent topological constraints that persist and strengthen with aging. While these results quantify threading at the level of pairwise ring interactions, an open question remains as to how such persistent topological constraints organize the system spatially at larger length scales. In particular, if threading acts as a dominant source of dynamical arrest, it could potentially lead to spatially heterogeneous organization of the centers of mass of the rings, reflecting collective entrapment. To address this, we examine the emergence and evolution of clusters in the spatial organization of ring polymers.

To characterize collective spatial organization, we analyze the clustering of ring COMs as the system is quenched from a high-temperature liquid state to temperatures in the glassy regime, i.e., $T < T_c$. We employ the DBSCAN algorithm to identify clusters; details of the method and parameters are provided in Appendix H. Figure 11 shows representative snapshots of the COM evolution and the corresponding virtual bonds between COMs. Two COMs are considered connected if the corresponding rings are threaded and the distance between them is less than the instantaneous average radius of gyration, $\langle R_g(t) \rangle$, where $\langle \cdot \rangle$ denotes an average over all rings at time t . Intercluster threaded rings are indicated by purple bonds. As evident from Fig. 11, a finite number of polymers thread with polymers belonging to different clusters, indicating nontrivial intercluster connectivity.

At $t = 0$, which is representative of the high-temperature state from where the thermal quench is initiated, there is spatial homogeneity and no clusters are observed [see Figs. 11(a) and 11(e)]. As the system undergoes thermal quench with time (from left to right in top and bottom panels of Fig. 11(h)), clusters begin to form progressively. Both the number and the size of clusters increase with time as the glassy state develops.

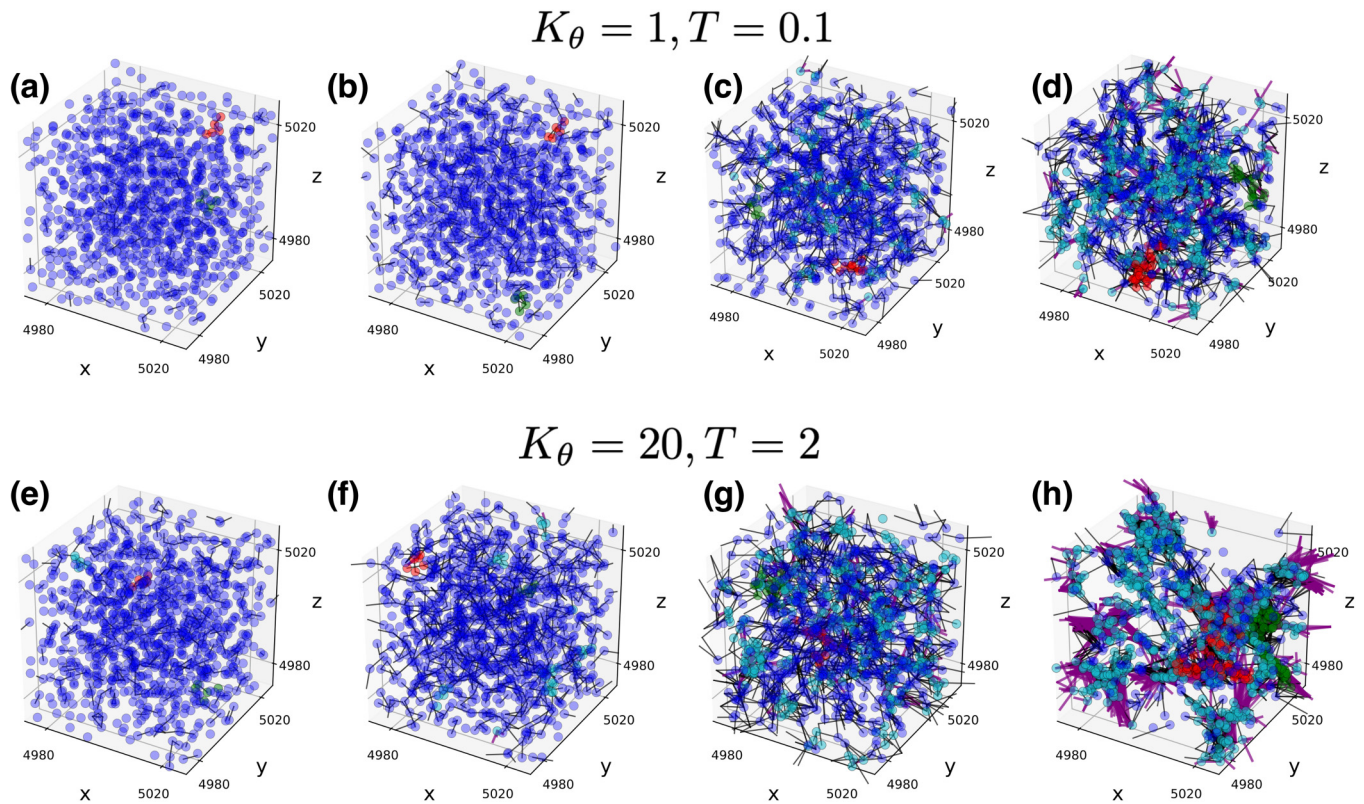


FIG. 11. Snapshots of the spatial organization of ring-polymer centers of mass at different times following a thermal quench. Panels (a)–(d) correspond to $K_\theta = 1$, $T = 0.1$, and panels (e)–(h) to $K_\theta = 20$, $T = 2$, shown at $t = 0\tau$, 183τ , $2.7 \times 10^4\tau$, and $1.5 \times 10^6\tau$, respectively. Blue spheres denote COMs not belonging to any cluster. Solid black lines indicate virtual-neighbor connections between threaded polymers. Purple lines indicate intercluster connections. The largest and second-largest clusters are highlighted in red and green, respectively.

We observe maximal clustering and ensuing spatial heterogeneity at temperatures near T_c (see bottom panel of Fig. 11). In contrast, at $T \ll T_c$, both the average cluster size and the number of clusters remain small (see top panel of Fig. 11). At these low temperatures, reduced thermal fluctuations slow down large-scale rearrangements, delaying cluster formation, and preserving homogeneity over longer times. For temperatures above T_c , clustering becomes less and less evidenced (see Fig. 25), as the rings adopt compact, soft-sphere-like conformations that increase the effective screening distance between COMs.

Polymer stiffness further modulates cluster formation. In Figs. 12(a) and 12(b), we plot the evolution of the average cluster size, $C_{av}^s(t)$, for different stiffness values, at the respective temperatures as indicated. A clear distinction emerges between flexible and rigid systems [see Fig. 12(a)]: Flexible systems ($K_\theta = 1, 5$) exhibit weaker clustering, whereas stiffer systems ($K_\theta = 10, 20$) display significantly larger clusters, highlighting the role of stiffness in enhancing collective organization of ring COMs. At the lower temperatures [see Fig. 12(b)], the clustering process gets arrested because of the lack of thermal fluctuations in initiating structural reorganizations.

To quantify cluster participation, we compute the fraction of polymers $f_c(t)$ that belong to a cluster at a given time. Clusters are defined as containing at least two members, excluding isolated single-particle clusters identified by the DBSCAN algorithm. As shown in Figs. 12(c) and 12(d), the

fraction of polymers participating in clusters increases upon quenching below T_c . The dependence of $f_c(t)$ on stiffness and temperature is presented in Figs. 12(c) and 12(d). Stiffer systems exhibit substantially higher cluster participation, with up to $\sim 80\%$ of polymers forming clusters in the final state, whereas flexible systems ($K_\theta = 1$) show reduced clustering, with a maximum participation of approximately 40%. At temperatures well below T_c , cluster participation decreases again [Fig. 12(d)].

A comparison of maximum cluster size and cluster participation across T_c is provided in Appendix H. Figure 26 summarizes the temperature dependence of clustering and shows that cluster formation is maximized near the transition temperature and suppressed both above and below it. Notably, this trend closely mirrors the temperature dependence of threading events [Figs. 8(d) and 8(e)], indicating a strong correlation between threading interactions and cluster formation. This correspondence suggests that persistent threading facilitates the collective caging of polymers and promotes the formation of spatially heterogeneous domains in topological glasses.

We now examine how aging influences the dynamics of cluster formation and evolution, using the two complementary measures discussed above: the average cluster size and the fraction of polymers participating in clusters. These quantities allow us to distinguish between aging effects associated with cluster restructuring and the incorporation of polymers into collective via increased clustering. Figures 13 shows the

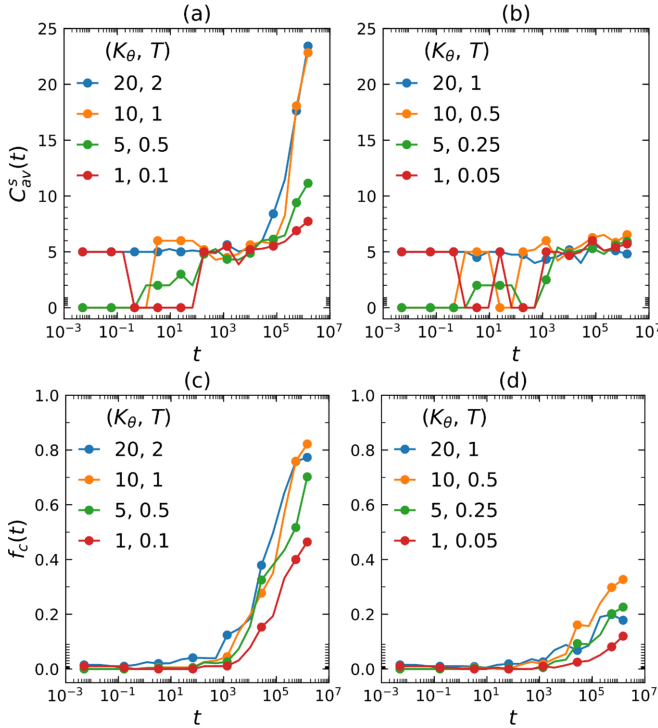


FIG. 12. Time evolution of the (a), (b) average cluster size, $C_{av}^s(t)$, (c), (d) fraction of polymers participating in clusters, $f_c(t)$, for different polymer stiffnesses at their respective temperatures as marked. The left panel corresponds to temperatures just below T_c , while the right panel shows results at the lowest temperature investigated in this study.

changes in the average cluster size, ΔC_{av}^s (top panel), and in the cluster participation fraction, Δf_c (bottom panel).

We first consider the evolution of the average cluster size. For rigid systems, ΔC_{av}^s exhibits no systematic dependence on the waiting time t_w . The curves display only weak, unsystematic fluctuations with age, indicating the absence of pronounced aging effects in cluster size. Instead, ΔC_{av}^s depends primarily on temperature at fixed stiffness [Figs. 13(a) and 13(b)]. At low temperatures, ΔC_{av}^s remains close to zero over the entire observation window, reflecting strong dynamical arrest. At higher temperatures, ΔC_{av}^s increases rapidly with time, consistent with enhanced mobility and restructuring of clusters, but still without exhibiting clear aging dependence.

The lack of aging in the average cluster size suggests that once clusters form, their typical size is largely determined by temperature rather than by the age of the system. In the deeply glassy regime, reduced thermal fluctuations suppress large-scale rearrangements, effectively freezing cluster sizes. Additional results for intermediate stiffness values ($K_\theta = 5, 10$) are shown in Fig. 27.

In contrast, the fraction of polymers participating in clusters exhibits a weak but systematic dependence on the waiting time. As shown in Figs. 13(c) and 13(d), Δf_c increases gradually with time. The growth is more pronounced at higher temperatures for a given stiffness, indicating that thermal fluctuations facilitate the incorporation of additional polymers into existing clusters. As the system ages, the rate of increase

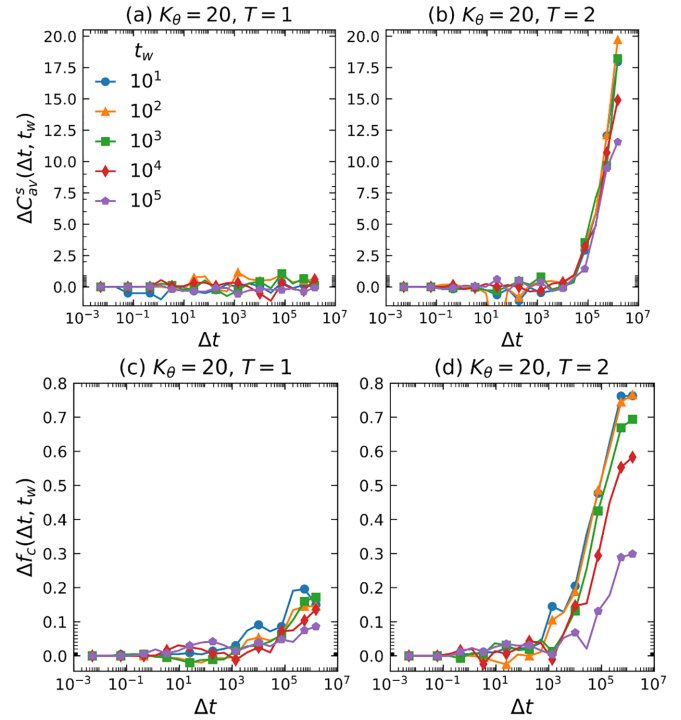


FIG. 13. Change in (a), (b) average cluster size $\Delta C_{av}^s(\Delta t, t_w)$, (c), (d) fraction of polymers participating in clusters $\Delta f_c(\Delta t, t_w)$, for different waiting times for $K_\theta = 20$.

of Δf_c slows down, signaling progressive dynamical arrest in cluster participation. This behavior reflects aging at the level of cluster membership rather than cluster size. Results for $K_\theta = 5, 10$ are provided in Fig. 28.

IV. SUMMARY AND DISCUSSION

In this study, we investigated the aging dynamics of dense, topologically constrained ring-polymer systems using large-scale molecular dynamics simulations. In the supercooled regime, we measure diffusion coefficient of the center of the mass of the polymer rings and use the temperature dependence of the diffusion coefficient to estimate the temperature (T_c) at which the diffusion of the rings is expected to vanish, i.e., the temperature below which the system would be nonergodic. We established that T_c increases steadily with polymer stiffness (K_θ). This highlights the role of rigidity in enhancing configurational constraints and increasing the energy barriers for relaxation. Such behavior is consistent with prior observations in linear-polymer systems and colloidal glasses, reinforcing the general principle that increased stiffness shifts the glass transition to higher temperatures.

Below T_c , characteristic features of aging are observed. Analysis of the two-time correlation functions, viz., mean-square displacement and self-intermediate scattering function, revealed a clear dependence on the waiting time t_w , which is a hallmark of aging behavior. The structural relaxation time τ_α , extracted from the self-intermediate scattering function, follows a sublinear power-law scaling, $\tau_\alpha \sim t_w^b$, consistent with simple aging scenarios reported in colloidal glasses.

A defining feature of ring-polymer melts is the occurrence of threading events, which introduce topological constraints absent in linear polymers. Upon thermal quench, the degree of threading increases as the system becomes dynamically arrested. The threading measure $\Delta(t)$ exhibits distinct stiffness-dependent behavior: Highly rigid rings ($K_\theta = 20$) show rapid saturation of threading due to strong topological constraints, whereas more flexible rings exhibit sustained growth of threading over long timescales, characterized by a power law $\Delta(t) \sim t^\eta$ with decreasing η as stiffness increases. These trends reflect the competing roles of conformational flexibility and excluded-volume constraints in enabling topological rearrangements.

Aging further amplifies the role of threading. Analysis of threading gain and loss demonstrates that, as the system ages, the formation of new threadings slows while existing threadings become increasingly persistent. This is captured quantitatively by the threading persistence function $\phi_p(t_w, t)$, whose decay slows systematically with increasing waiting time. The corresponding threading relaxation timescale $\tau_d(t_w)$ exhibits a power-law dependence on t_w similar to that of τ_α , establishing a direct correspondence between topological and structural relaxation. These results identify threading as the dominant slow variable governing aging in ring-polymer glasses.

The persistence of threading interactions has direct consequences for polymer conformations and spatial organization. Shape analysis reveals pronounced aging effects: Rigid rings undergo late-time shape relaxation near T_c , whereas flexible rings saturate earlier. The radius of gyration increases with age and does not relax back at long times, indicating a gradual evolution toward more open, disklike conformations that are conducive to threading. These conformational changes further stabilize topological constraints and reinforce dynamical arrest. At the collective level, persistent threading gives rise to pronounced spatial heterogeneity, manifested as clustering of ring centers of mass. Cluster analysis reveals that both cluster size and number depend strongly on temperature and stiffness. Clustering is maximized near the transition temperature, where polymer mobility and long-lived threading coexist. At low temperatures, cluster growth is inhibited by deep dynamical arrest, whereas at high temperatures, thermal fluctuations destabilize threading-mediated contacts. Stiffer rings exhibit stronger clustering than flexible systems, reflecting their enhanced ability to sustain long-lived threadings. These observations establish cluster formation as a spatial footprint of topological constraints in glassy ring-polymer systems.

Overall, our results reveal a coherent picture in which polymer stiffness controls the onset of dynamical arrest, threading events act as long-lived topological constraints that govern aging, and clustering emerges as the spatial manifestation of these constraints. The interplay between stiffness, topology, and aging produces a form of slow dynamics distinct from conventional polymeric and colloidal glasses, highlighting the crucial role of polymer architecture in shaping nonequilibrium behavior. Future studies on mixed-topology or polydisperse ring systems may further elucidate how heterogeneity in threading influences macroscopic aging and relaxation pathways.

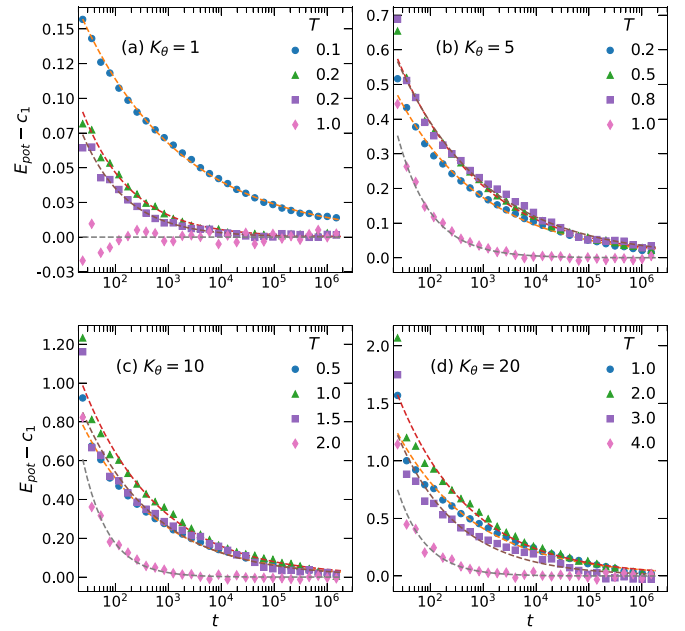


FIG. 14. Time variation of potential energy for various polymer stiffness K_θ . The energy is fitted (dashed line) to the algebraic function $E_{\text{pot}} = a_1 t^{-b_1} + c_1$ and shifted by its intercept (c_1).

ACKNOWLEDGMENTS

We thank the HPC facility at The Institute of Mathematical Sciences for computing time. P.C. and S.V. also acknowledge support via the subproject on the Modeling of Soft Materials within the IMSC Apex project, funded by Department of Atomic Energy.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

TABLE I. b_1 and b_2 values obtained from algebraic fit $E_{\text{pot}} \sim t^{-b_1}$ (refer to Fig. 2) and logarithmic fit $E_{\text{pot}} \sim (\log_{10}(t))^{-b_2}$. Here, $T_1 < T_2 < T_3 < T_4$, and T_i 's are temperature values used for each K_θ 's in Figs. 14 and 15.

	b_1			
	$K_\theta = 1$	$K_\theta = 5$	$K_\theta = 10$	$K_\theta = 20$
T_1	0.23	0.26	0.30	0.30
T_2	0.47	0.27	0.30	0.31
T_3	0.52	0.26	0.32	0.38
T_4	0.99	0.69	0.88	0.81
	b_2			
	$K_\theta = 1$	$K_\theta = 5$	$K_\theta = 10$	$K_\theta = 20$
T_1	0.58	0.83	1.05	1.04
T_2	1.8	0.87	1.06	1.15
T_3	2.0	0.83	1.2	1.58
T_4	5.0	2.8	2.45	2.27

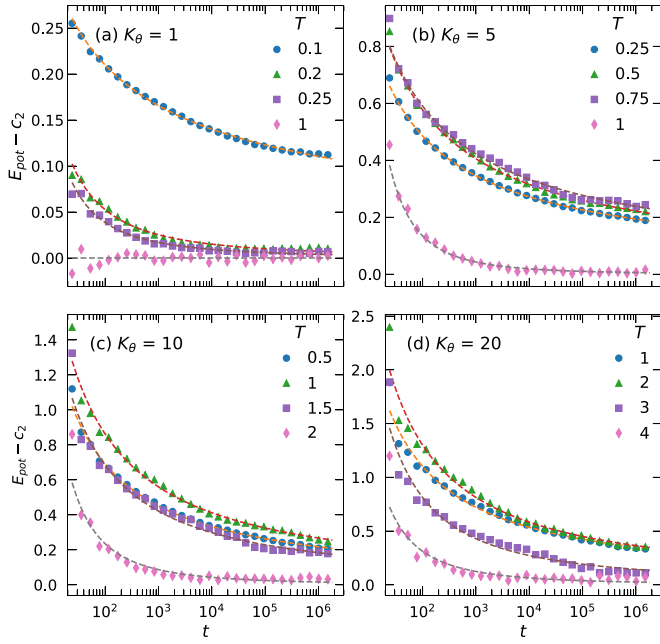


FIG. 15. Time variation of potential energy for various polymer stiffness K_θ . The energy is fitted (dashed line) to the algebraic function $E_{\text{pot}} = a_2[\log(t)]^{-b_2} + c_2$ and shifted by its intercept (c_2).

APPENDIX A: POTENTIAL ENERGY DURING QUENCH

Figure 14 shows the evolution of potential energy immediately after the quench ($t = 0$). In the supercooled regime, E_{pot} decreases initially and subsequently reaches a plateau, corresponding to its equilibrium value at that temperature. Conversely, in the glassy regime, the potential energy fails to attain a steady-state plateau within accessible simulation timescales. Figure 14 presents the time evolution of E_{pot} for different temperatures and polymer stiffness values, illustrating the stiffness-dependent variation in glass transition temperature. For flexible polymers ($K_\theta = 1$), we note that the onset of glassy dynamics occurs around $T \approx 0.1$, where E_{pot} does not stabilize within our observation window. Semiflexible polymers ($K_\theta = 5$) show glassy behavior at $T \approx 0.75$ but equilibrate at $T = 1$, indicating a slightly higher glass transition temperature compared to flexible polymers.

For rigid polymers ($K_\theta = 10, 20$), we progressively observe higher transition temperatures, with clear out-of-equilibrium dynamics emerging at $T \approx 1.5$ for $K_\theta = 10$ and at $T \approx 3$ for $K_\theta = 20$. To quantitatively characterize these relaxation dynamics, we fit the potential-energy curves using the algebraic form $E_{\text{pot}} = a_1 t^{-b_1} + c_1$ (dashed lines in Fig. 14); here, energy curves are shifted by c_1 to facilitate direct comparison. The fitting parameter b_1 serves as an indicator of structural relaxation timescales, with values between 0.2 and 0.4 representing slow relaxation typical of glassy systems, whereas $b_1 > 0.4$ corresponds to the nonglassy regime; see Table I for details on the obtained fit values.

In Fig. 15, we present logarithmic fits to the potential-energy curves using the form $E_{\text{pot}} = a_2[\log(t)]^{-b_2} + c_2$. The extracted exponent b_2 (see Table I) ranges from 0.4 to 5 across the various temperatures and K_θ values considered. For glassy systems, values of $b_2 < 2$ indicate a slow decay in potential energy, consistent with slow relaxation. A similar trend is observed in the exponent b_1 from the algebraic fits (see Fig. 2), with larger exponents corresponding to faster decay, typical of nonglassy systems that relax rapidly to equilibrium. As the temperature decreases and the system approaches the glassy regime, both exponents decrease, reflecting slower potential-energy relaxation. Notably, flexible polymers ($K_\theta = 1$) exhibit a sharp increase in b_1 and b_2 , attributed to enhanced configurational entropy that accelerates relaxation. In contrast, semiflexible and rigid polymers show significantly slower decay due to increased effective volume and reduced configurational entropy. Overall, this analysis delineates the thermal regimes corresponding to out-of-equilibrium dynamics for different values of K_θ , setting the stage for subsequent exploration of aging phenomena [48,51].

APPENDIX B: MEAN-SQUARE DISPLACEMENT

Figure 16 shows the MSD curves for $K_\theta = 5, 10, 15$. As the stiffness of the polymer backbone increases, the onset of the diffusive regime progressively shifts to higher temperatures. This trend reflects the increasing configurational constraints imposed by enhanced chain rigidity. For highly stiff polymers, such as $K_\theta = 15$, diffusive behavior is observed only at higher temperatures ($T \approx 6$), consistent with the behavior reported for $K_\theta = 20$ (see main text).

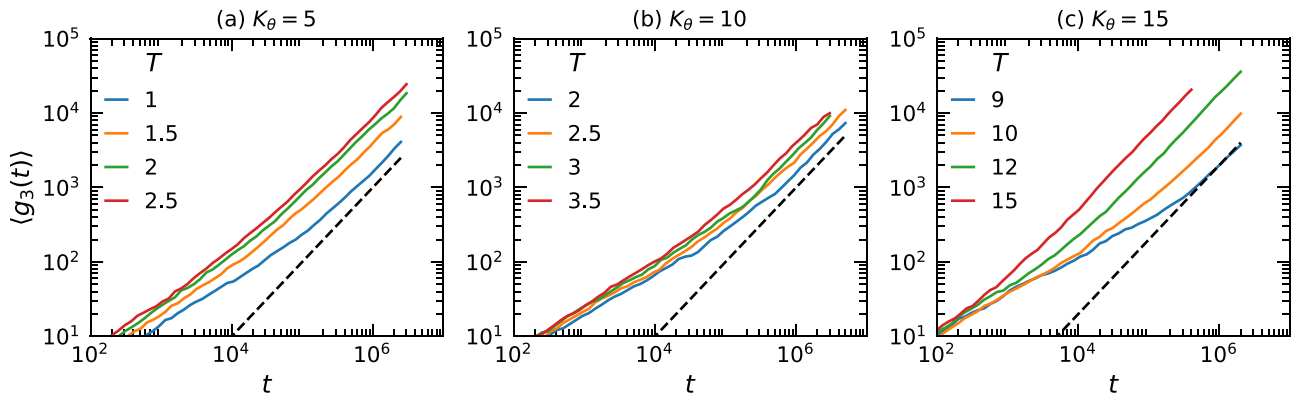


FIG. 16. Mean-square displacement of the center of mass of polymers, $\langle \Delta r^2(t) \rangle$, for various K_θ values. Here, the $\langle \cdot \rangle$ represents the average over all rings. t is the time since the thermal quench.

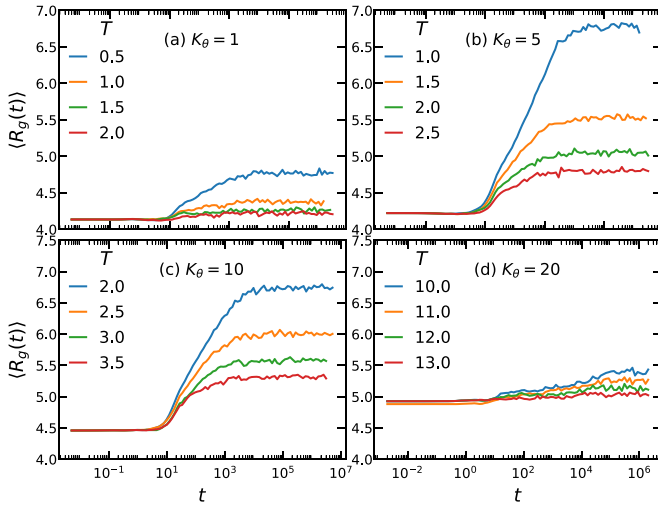


FIG. 17. Evolution of mean radius of gyration after the quench. Panels (a)–(d) represent $\langle R_g(t) \rangle$ for $K_\theta = 1, 5, 10, 20$, respectively, at different temperature values (see legends).

The diffusion curves in Fig. 2(c) clearly demonstrate that for $K_\theta > 10$, the system dynamics slow down considerably, which can be attributed to the increased effective volume associated with the rigid polymer structure, which further limits configurational rearrangements. As a result, the characteristic temperature at which diffusion emerges shifts to higher values for stiffer polymers.

APPENDIX C: RADIUS OF GYRATION

The structural properties of ring polymers play an important role in topological glasses, where an open and extended polymer facilitates more threading events leading to a dynamical arrest of the system. On the other hand, crumpled and compact ring configurations lead to lesser threading events resulting in a liquid phase. In this section, we show the average radius of gyration for various stiffness and temperatures as a function of time. Upon quenching the system from high to low temperature, we observe an initial increase in the mean radius of gyration, which eventually saturates, signaling the approach to an equilibrium phase.

The radius of gyration depends on both the stiffness of the polymers and the system temperature. Stiff polymers tend to adopt extended configurations in order to minimize bending energy, whereas at higher temperatures, polymers can assume crumpled conformations as thermal fluctuations help overcome the bending potential. This trend is evident in Fig. 17, where we observe an increase in the mean radius of gyration as the temperature is lowered for a fixed stiffness. Conversely, for a fixed temperature, increasing the stiffness leads to a larger equilibrium value of $\langle R_g \rangle$, consistent with the tendency of stiffer polymers to take extended structures.

APPENDIX D: SHAPE ANISOTROPY AND THREADING

In our simulations, rings with a comparable number of threaded polymers exhibit distinct behaviors, i.e., some escape the caging, while others remain trapped. Especially, rings with twisted or folded conformations tend to stay confined and fail to break the cage. To quantify the role of polymer shape in

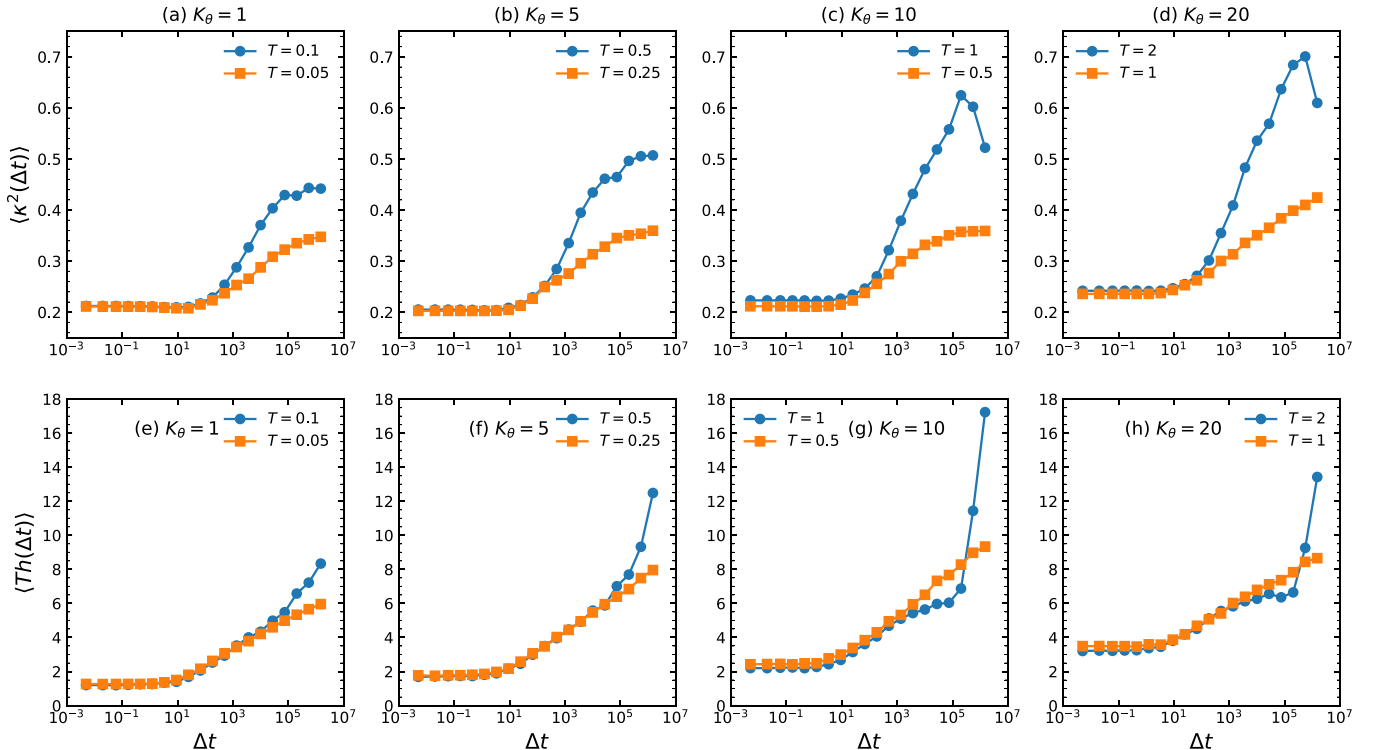


FIG. 18. Upper panel: time series of average anisotropy $\langle \kappa^2(\Delta t) \rangle$ of the polymers for various stiffness and temperatures. Lower panel: the corresponding time evolution of average number of threaded polymers to a polymer. Here, the waiting time $t_w = 10$.

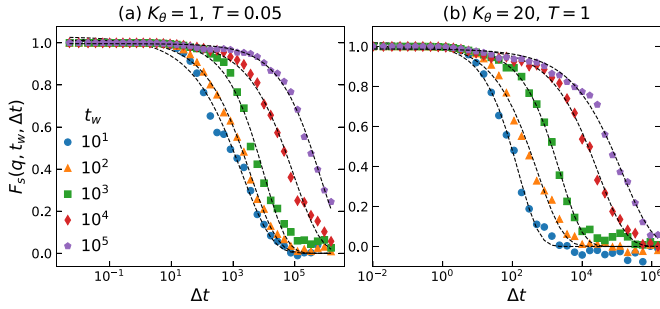


FIG. 19. ISF curves for $K_\theta = 1, 20$, at $T = 0.05$ and 1 , respectively. Here, $|q| = 1$.

this slowdown, we evaluate the relative shape anisotropy of the rings (Fig. 18), defined from the gyration tensor as [52,53]

$$\kappa^2 = \frac{3}{2} \frac{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}{(\lambda_1 + \lambda_2 + \lambda_3)^2} - \frac{1}{2}. \quad (\text{D1})$$

Where $\lambda_1 < \lambda_2 < \lambda_3$ are the eigenvalues of the gyration tensor. The parameter $\kappa^2 \in [0, 1]$, with $\kappa^2 = 0$ for isotropic (spherical) and $\kappa^2 = 1$ for linear (rodlike or doubly folded) conformations. In the ideal limit, $\kappa^2 \rightarrow 1$ corresponds to vanishing threading ($\text{Th} \rightarrow 0$).

Figure 18 compares the average anisotropy $\langle \kappa^2 \rangle$ and the average number of threaded polymers $\langle \text{Th} \rangle$. At high temperatures, the rings are crumpled with $\langle \kappa^2 \rangle \approx 0$. The initial plateau is due to the transient high-temperature effect after the quench. After the temperature settles at the target temperature ($T < T_c$), the polymers expand to minimize bending energy, becoming more anisotropic and increasing their elastic modulus κ^2 . The threading dynamics follow a similar trend: As rings evolve from compact to extended conformations, the number of threading events increases, reflecting the correlation between anisotropy growth and the threading process.

At longer times ($t > 10^5$), $\langle \kappa^2 \rangle$ plateaus at temperatures lower than the transition temperature ($T < T_c$). In contrast, for temperatures closer to the transition temperature

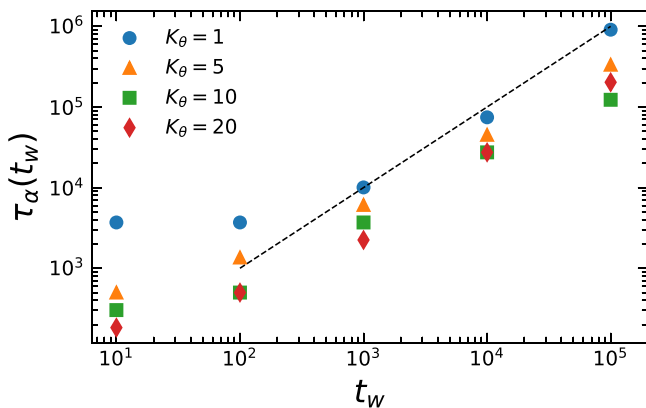


FIG. 20. Relaxation time (τ_α) as a function of waiting time (t_w) for $K_\theta = 1, 5, 10$, and 20 , at temperatures $T = 0.05, 0.25, 0.5$, and 1 , respectively.

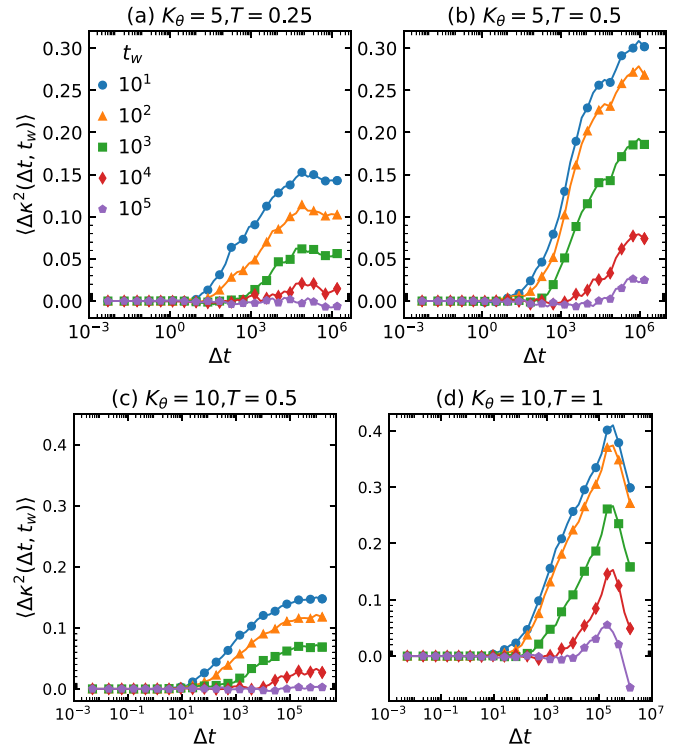


FIG. 21. Change in relative shape anisotropy $\langle \Delta \kappa^2(\Delta t, t_w) \rangle$ for different waiting times below the glass transition temperature. Upper panels correspond to rigid rings ($K_\theta = 20$) and lower panels to flexible rings ($K_\theta = 1$). The $\langle \cdot \rangle$ represent the average over all rings.

($T \approx T_c$), the long-time behavior of $\langle \kappa^2 \rangle$ shows an overall decline. Interestingly, the number of threading events, $\langle \text{Th} \rangle$, continues to rise. In each case considered here [Figs. 18(e)–18(h)], temperatures closer to T_c show a sharp increase in threading events (e.g., for $K_\theta = 10, T = 1$) at times $t > 10^5$. For such cases, we observe a decline in the corresponding relative shape anisotropy curve at times $t > 10^5$, suggesting a deviation of rings from a doubly folded linear shape toward more open configurations, facilitating additional threading, which can be a possible explanation for the sharp rise in threading events at temperatures close to T_c . Whereas, at lower temperatures ($T \ll T_c, K_\theta = 10, T = 0.5$), polymers are more compact, and the lack of thermal energy excludes the possibility of long-time relaxation, leading to fewer threading events per ring.

APPENDIX E: INTERMEDIATE SCATTERING FUNCTION DURING AGING

In this section, we show the aging effect on the intermediate scattering function for two contrasting stiffness values $K_\theta = 1$ and 20 for different waiting times (see Fig. 19). The flexible ($K_\theta = 1$) and rigid ($K_\theta = 20$) systems show aging behavior at their respective temperatures, with flexible system showing a higher relaxation time compared to the rigid system, due to reduced motility as a result of its flexibility (see Fig. 19). In Fig. 20, We compare the relaxation time across various stiffness values at different temperatures. It is evident that the flexible systems ($K_\theta = 1, 5$) show larger

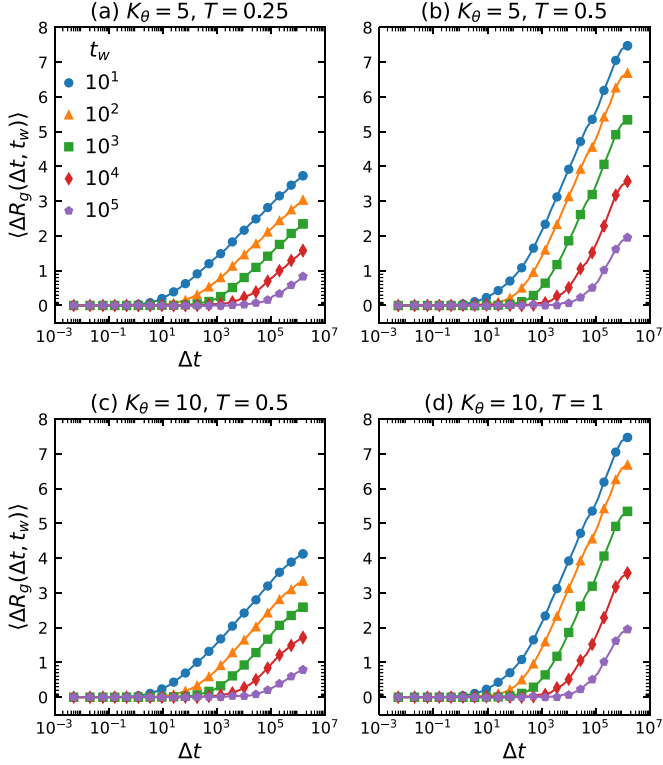


FIG. 22. Change in radius of gyration $\langle \Delta R_g(\Delta t, t_w) \rangle$ for different waiting times. Results are shown for rigid and flexible systems at temperatures close to their respective glass temperatures. The $\langle \cdot \rangle$ represent the average over all rings.

relaxation time than their rigid counter parts due to reduced rigidity impacting its structural rearrangements. Note that the temperatures considered in this plot corresponds to $T \approx T_c/2$ for all stiffness values except $K_\theta = 20$, for which $T \approx T_c/7$.

APPENDIX F: AGING EFFECT ON RING CONFORMATION

In this section, we report the effect of aging on ring conformation. In Fig. 22, we plot the change in relative anisotropy for $K_\theta = 5, 10$. In both cases, we observe an increase in $\Delta\kappa^2$ over the temperature range considered here. The semi-flexible system ($K_\theta = 5$) shows a saturation in $\Delta\kappa^2$ at long times. In contrast, the stiffer system exhibits a decline in $\Delta\kappa^2$ at long times, similar to the behavior observed for stiff polymers in Fig. 6. These results suggest that stiffer systems ($K_\theta \geq 10$) undergo a doubly folded linear-to-disk transition at temperatures close to the transition temperature. The consequences of this transformation are reflected in the increase in the number of threading events shown in Fig. 18(e)–18(h).

Next, we examine the effect of aging on the change in the radius of gyration of the rings for $K_\theta = 5, 10$. Similar to the flexible and rigid cases shown in Fig. 7 of the main text, we observe an increase in ΔR_g with increasing observation time. In addition, as the waiting time increases, the onset of the increase in ΔR_g shifts to longer times. Unlike the behavior of $\Delta\kappa^2$, however, no decline in ΔR_g is observed at long times.

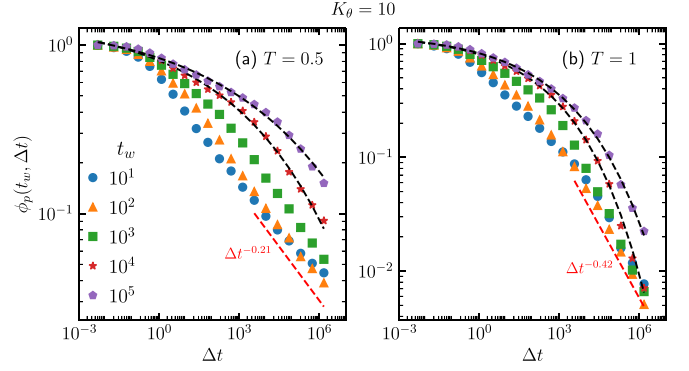


FIG. 23. Aging effect on threading correlation function (see main text for definition) for $K_\theta = 10$ and different temperature values. The black-dashed line is a fit to the stretched-exponential function $\phi_p(t_w, \Delta t) \sim e^{-(\Delta t/\tau_p)^{\beta_p}}$. For small waiting times ($t_w = 10$), the region $\Delta t > 10^3$ is fit with $\phi_p(t_w, \Delta t) \sim \Delta t^{-\xi}$, represented by the red dashed line.

APPENDIX G: THREADING CONTIGUITY

In Fig. 23, we fit the threading correlation function ϕ_p to a stretched exponential to extract the relaxation behavior of unthreading events for $K_\theta = 10$. At low t_w , the curves show fat tails and deviate from the stretched exponential, indicating a slower decay in ϕ_p . Fitting the tail region ($\Delta t > 10^3$) for $10 \leq t_w \leq 1000$ to an algebraic form $\Delta t^{-\xi}$ confirms this slower decay, with ξ ranging from 0.17 to 0.23 for $T = 0.5$ and 0.38 to 0.48 for $T = 1$. The tail decay in ϕ_p is notably slower than the coil-coil contiguity correlation reported in Ref. [50], where the tail exponent $\xi \approx 3/4$. The stretching exponent β_p lies between 0.1 and 0.2, much lower than typical ISF values ($\beta > 0.4$). While fat tails appear at smaller t_w , they disappear at higher t_w , indicating a crossover from a tail-dominated slow decay to a slower stretched-exponential relaxation. However, for highly rigid systems, fat-tail dominated decay persists even for higher t_w [Fig. 24(b)].

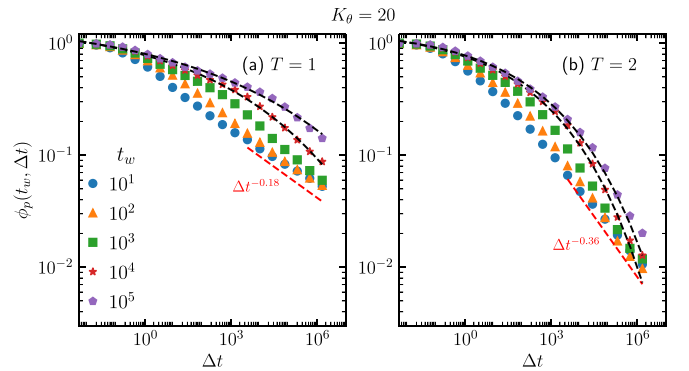


FIG. 24. Aging effect on threading correlation function (see main text for definition) for $K_\theta = 20$ and different temperature values. The black dashed line is a fit to the stretched-exponential function $\phi_p(t_w, \Delta t) \sim e^{-(\Delta t/\tau_p)^{\beta_p}}$. For small waiting times ($t_w = 10$), the region $\Delta t > 10^3$ is fit with $\phi_p(t_w, \Delta t) \sim \Delta t^{-\xi}$, represented by the red dashed line.

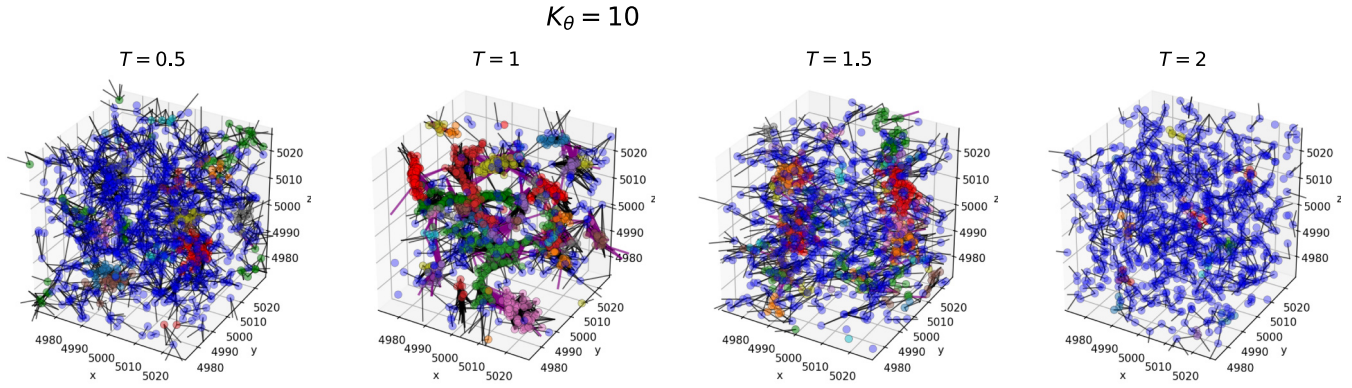


FIG. 25. Comparison of clusters for $K_\theta = 10$ at various temperatures above and below the transition temperature ($T_c \approx 1$). The snapshots correspond to the final configuration in each case ($t = 1\,500\,000$, τ). Blue circles represent noise, i.e., COMs that are not part of any cluster. The largest and second-largest clusters are shown in red and green, respectively. Black lines indicate virtual bonds (see main text for definition), while purple lines denote intercluster virtual bonds, i.e., bonds between particles belonging to different clusters.

APPENDIX H: CLUSTER FORMATION AND BOND NETWORK ANALYSIS

1. DBSCAN method

In this section, we describe the density-based spatial clustering of applications with noise (DBSCAN) algorithm used to identify clusters in our system. DBSCAN is a density-based, unsupervised clustering method [54]. The analysis was performed using the `scikit-learn` library in Python [55].

DBSCAN requires two key parameters: the neighbourhood radius ϵ and the minimum number of points $n_{\min}$ within the radius. A particle is classified as a core point if at least $n_{\min}$ particles lie within a distance ϵ . In our analysis, particles correspond to ring's center of mass. We fix $\epsilon = 4$ and $n_{\min} = 5$ for our system. Pairwise distances are computed using the minimum-image convention to account for periodic boundary conditions [56]. The algorithm identifies cluster members and cluster sizes, while particles not assigned to any cluster are labeled as noise (blue circles in Fig. 25). We track the average cluster size and the fraction of polymers participating in clusters at each time. In this section, we show the clustering across the transition temperature T_c for $K_\theta = 10$. Figure 25

shows snapshots of COMs at different times for $K_\theta = 10$ and various temperatures at and above the transition temperature, $T_c \approx 1$. The two largest clusters are highlighted in red and green, respectively. As seen in Fig. 25, the cluster formation is most pronounced around the transition temperature. Moreover, clustering does not disappear abruptly at T_c but decreases gradually with increasing temperature.

To quantify this behavior across the transition temperature, we plot the maximum cluster size and the fraction of polymers

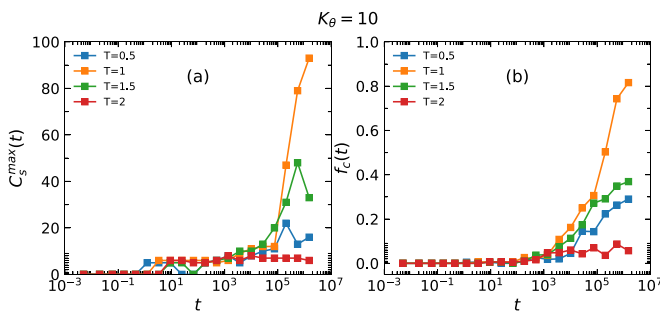


FIG. 26. Evolution of (a) the maximum cluster size and (b) the fraction of polymers forming clusters for $K_\theta = 10$ at temperatures above and below the transition temperature ($T_c \approx 1$).

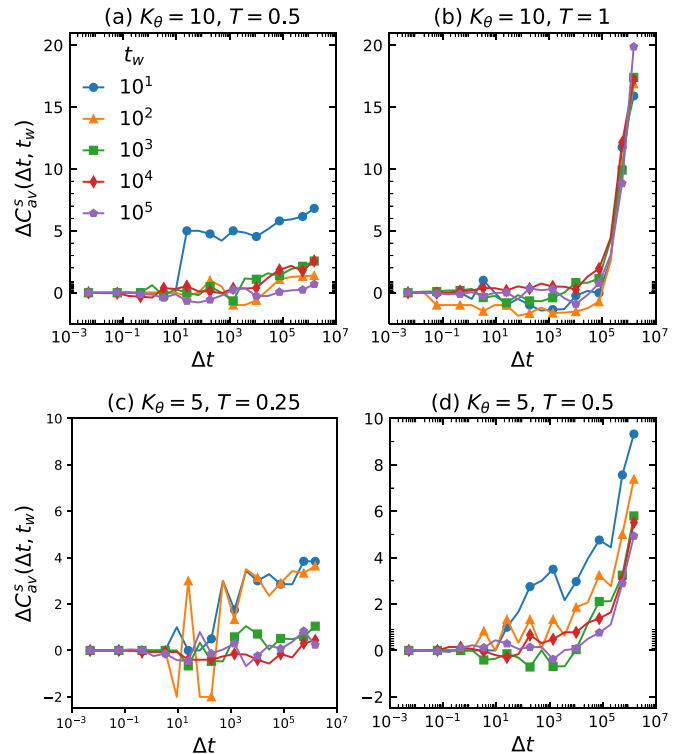


FIG. 27. Change in average cluster size relative to different waiting times.

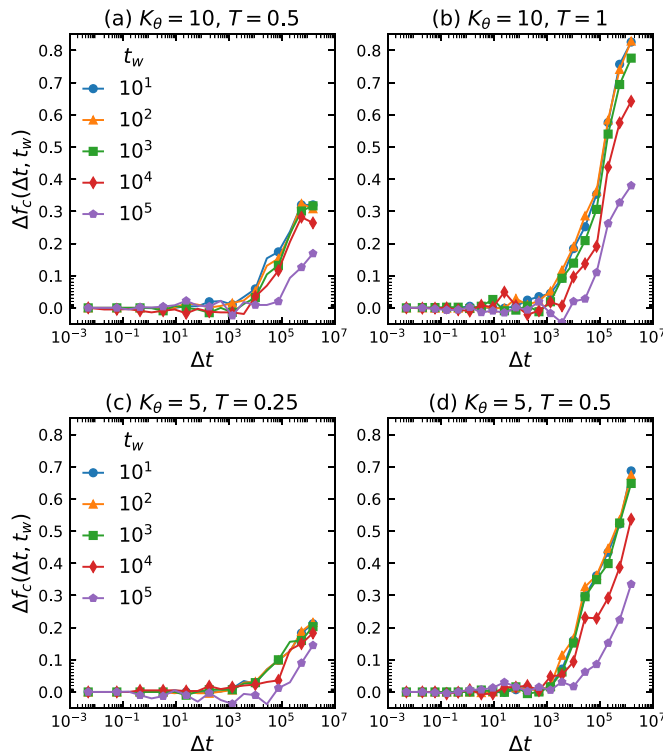


FIG. 28. Change in fraction of polymers in clusters relative to different waiting times.

participating in clusters for $K_\theta = 10$, in Figs. 26(a) and 26(b). The maximum cluster size increases sharply for systems near $T_c \approx 1$, reaching about 100 polymers, i.e., roughly 10% of the polymers. At temperatures far from T_c , for instance $T = 0.5$ and $T = 2$, clustering is minimal. Similarly, the fraction of polymers forming clusters goes up after the quench

and is maximum at the transition temperature, with approximately 80% of the polymer forming clusters of size ≥ 2 . Further, for systems with temperatures farther from T_c , the participation of polymers in cluster formation goes down. Interestingly, this analysis is consistent with the threading analysis we observed earlier in Figs. 18(e)–18(h) (circles), where the threading events are maximum for systems with temperature $T \approx T_c$.

2. Aging effects on cluster dynamics

In this section, we report the effect of aging on the cluster dynamics of the system for $K_\theta = 5, 10$. Similar to Fig. 13 in the main text, the change in the average cluster size at lower temperatures ($T \approx 0.5$) shows weak but negligible age-dependent behavior for $K_\theta = 10$ (see Fig. 27(a)). However, at temperatures close to the transition temperature ($T \approx 1$), no systematic dependence on the age of the system is observed (see Fig. 27(b)). These results suggest that the cluster dynamics remain largely unaffected by the age of the system and that no large-scale rearrangement occurs after the formation of the initial clusters. Similarly, for $K_\theta = 5$, we observe very weak age dependence at short waiting times, and once the system enters a deep glassy state, cluster growth becomes arrested due to weak thermal fluctuations (see Fig. 27(c), 27(d)).

Unlike the average cluster size, the change in the fraction of polymers participating in cluster formation shows a weak but systematic age dependence. For both $K_\theta = 5$ and 10, we observe very weak age dependence at low temperatures, but a noticeable and systematic age dependence at higher temperatures (see Fig. 28(b), 28(c)). For short waiting times, the change in the fraction of polymers participating in cluster formation is significant. In contrast, as the waiting time increases and dynamic arrest sets in, fewer polymers participate in cluster formation due to low thermal energy.

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