

coordination number Z_j which only counts those contacts with nonzero forces. By definition $z_g \geq Z_j$.

While Z_j is easy to measure in computer simulations of soft particles as the number of contacts between overlapping particles, the geometrical coordination number, z_g , can be measured by slightly inflating the spheres up to 4% of their diameters and counting the resulting contact particles, as discussed in [7]. In practice, the geometrical coordination number measures the particles surrounding a central one with a gap between them from zero or negative (giving Z_j) up to $\delta = 0.08R$ as discussed in [7]. We notice that $\delta = 0.08R$ is much smaller than the location of the second peak in the radial distribution function which occurs around $\delta \sim 2R$. The value $\delta = 0.08R$ is specific for a system of $N=10,000$. We expect this value to diminish in the thermodynamic limit.

Figure 5B plots the geometrical and mechanical coordination z_g and Z_j as a function of ϕ_j for the same packings as in Fig. 1. We find that along the disordered branch, $z_g \approx Z_j$ as expected [7]. However, in the coexistence region, $Z_j = 6$ stays constant while z_g keeps growing with ϕ_j . The separation between z_g and Z_j is a signature of the onset of ordering at the freezing point. As explained above, the system starts to crystallize by allowing particles in the second coordination shell to come closer to the central particle and moving the Z_j contacting particles towards a FCC arrangement. At the melting point, the condition $Z_j = 6$ cannot hold any longer and the system transitions to the other branch with an increase of Z_j up to 12.

The distinction between z_g and Z_j is not only important for a characterization of the transition. It is also important to interpret the experimental results. Due to the uncertainty in detecting the exact position of the particles in any experiment, the exact mechanical coordination might be very difficult to obtain. Thus, a small uncertainty in the determination of the contacting particles $\delta = 0.08R$ will produce z_g as shown in Fig. 5B. One way to obtain the actual mechanical coordination from experimental data is to use the experimentally obtained coordinates of the particles as initial positions of a MD simulation using Hertz-Mindlin forces to relax the configurations and find the exact force balance network of the packing. Codes to develop this procedure are available at www.jamlab.org. We also provide most of the packings used in this study as well as the code to calculate the entropy.