the calculation of the Hessian matrix of the system at any time step. The PEL for each fixed ϕ likely includes millions of geometrically distinct minima by our simulation results. Therefore, an exhaustive search of configurations is computationally long. We check that the number of found configurations has saturated after sufficient trials such that the density of states $g(\Gamma, \phi)$ has converged to a final shape.

It is also important to determine if the local minima are distinct. Usually, the eigenvalues of the Hessian matrix at each local minimum can be used to distinguish these mechanically stable packings. Here, we follow this idea to compare minima to filter the symmetric packings. However, instead of calculating the eigenvalues of each packing, which is very time consuming, we calculate a function of the distance between any two particles in the packing to improve search efficiency (for the LBFGS algorithm, we do not need to calculate the Hessian matrix). For each packing, we assign the function Q_i for each particle in the system:

$$Q_i = \sum_{1\leq j\leq N,\ \ j\neq i} \tan^2(\frac{\pi r_{ij}^2}{3L^2}), \tag{14}$$

where r_{ij} is the distance between particles i and j, L is the system size and $N = 30$ is the number of the particles of the system. We list the Q_i for each packing from minimum to maximum $\{Q_i\}(1 \leq i \leq N)$. Since Q_i is a higher order nonlinear function, we can assume that two packings are the same if they have the same list. The tolerance is defined as:

$$T = \sqrt{\frac{\sum_{1\leq i\leq N}(Q_i - Q_i')^2}{N^2}}, \tag{15}$$

where Q_i and Q_i' are the corresponding values from the lists of two packings.

Figure 5 shows the distributions of the tolerance T for packings at different volume fractions. This figure suggests that two packings can be considered the same if $T \leq 10^{-1}$, which defines the noise level.

From Fig. 6, we see that after one week of searching, $g(\Gamma, \phi)$ does not change significantly, since the initial packings are generated by a completely random protocol. We also check the probability (defined as $\frac{N_{\text{new}}(i)}{N_{\text{total}}(i)}$, where $N_{\text{new}}(i)$ is the number of new configurations found on the ith day and $N_{\text{total}}(i)$ is the total number of configurations found in i days) of finding new mechanically stable states for different searching days. From Fig. 7, we see that, after one week searching, the probability of finding new configurations at different volume fractions converges, suggesting that enough ensemble packings have been obtained to capture the features of $g(\Gamma, \phi)$. A further test of convergence is obtained below in Fig. 11.