

Supplementary Information

Nucleation pathway and kinetics of phase-separating active Brownian particles

David Richard,¹ Hartmut Löwen,² and Thomas Speck¹

¹*Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7-9, 55128 Mainz, Germany*

²*Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany*

I. BASIN A AND FIRST INTERFACE

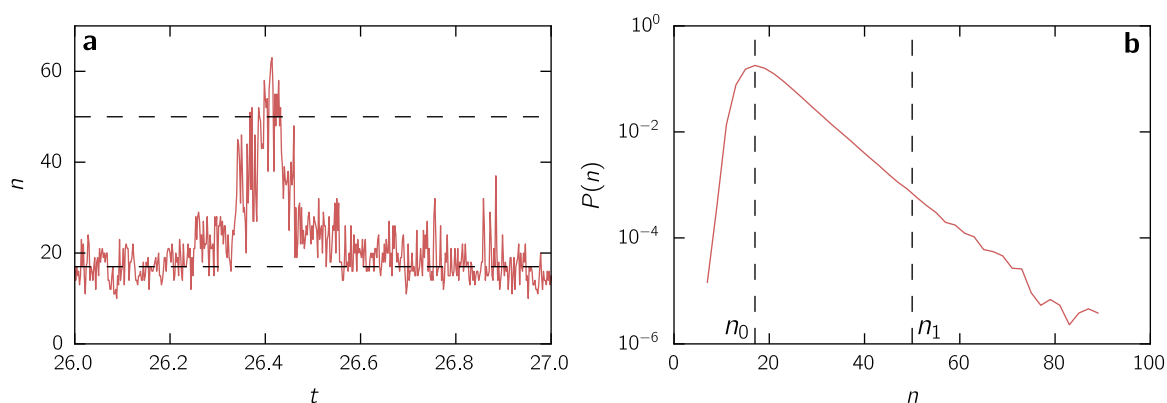


FIG. 1: Procedure to determine n_0 and n_1 . (a) Typical behavior of the order parameter n as a function of time t for one crossing event of the first interface. (b) Probability distribution $P(n)$ in the homogeneous phase and associated interface positions n_0 and n_1 for $\phi \simeq 0.23$. The position n_0 corresponds to the peak of the distribution whereas n_1 is determined by the probability to reach $\simeq 10^{-3}$.

II. CRITICAL NUCLEI SIZE

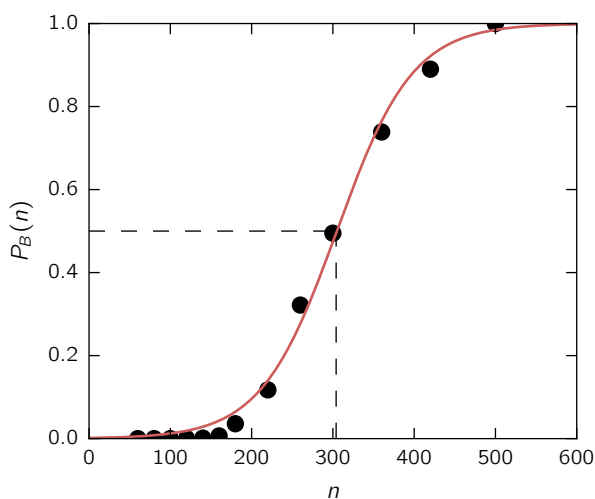


FIG. 2: Procedure to determine the size n_* of critical nuclei from the FFS data. Evolution of the forward transfer probability $P_j = \prod_{i=j}^{M-1} P(n_{i+1}|n_i)$ for one FFS run at $\phi \simeq 0.25$. The red solid line is a fit to the function $P(n) = \frac{1}{2}[1 + \tanh(cn + d)]$. The black dashed lines correspond to the TSE with $P_B = 1/2$ ($r_* = 0$) yielding $n_* = -d/c$.

| ϕ | c | d | n_* |
|--------|--------|--------|-------|
| 0.29 | 0.0145 | -3.519 | 243 |
| 0.27 | 0.0125 | -3.336 | 267 |
| 0.25 | 0.0120 | -3.610 | 301 |
| 0.23 | 0.0114 | -3.863 | 339 |

TABLE I: Parameters c and d extracted from FFS transfer probabilities (see Fig. 2) averaged over three independent runs.

III. LIKELIHOOD

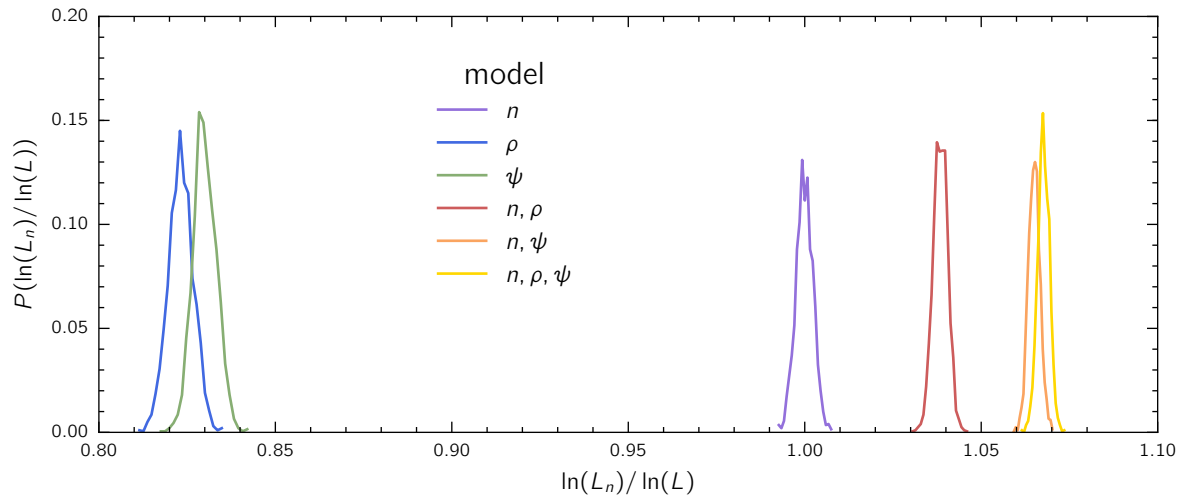


FIG. 3: Uncertainty of the log-likelihood. Distributions of $\ln(L_n)/\ln(L)$ extracted by the bootstrap method for the six different models. The procedure to evaluate an error of the maximum log-likelihood consists of resampling our data (each P_B) with an added Gaussian noise. The new set of P_B gives us a new log-likelihood, and this procedure is repeated 2000 times to get a distribution of $\ln(L)$. The variance of the noise is chosen to be equal to the variance of the residual $P_B(r_i) - P_B^m(r_i)$ computed between the data and the initial set of model parameters extracted from the likelihood maximization.