

## Supplementary Figures for Microscopic origin of tunable assembly forces in chiral active environments

Clay H. Batton and Grant M. Rotskoff\*

*Department of Chemistry, Stanford University, Stanford, CA, USA 94305*

(Dated: May 2, 2024)

### Appendix A: Supplementary Figures

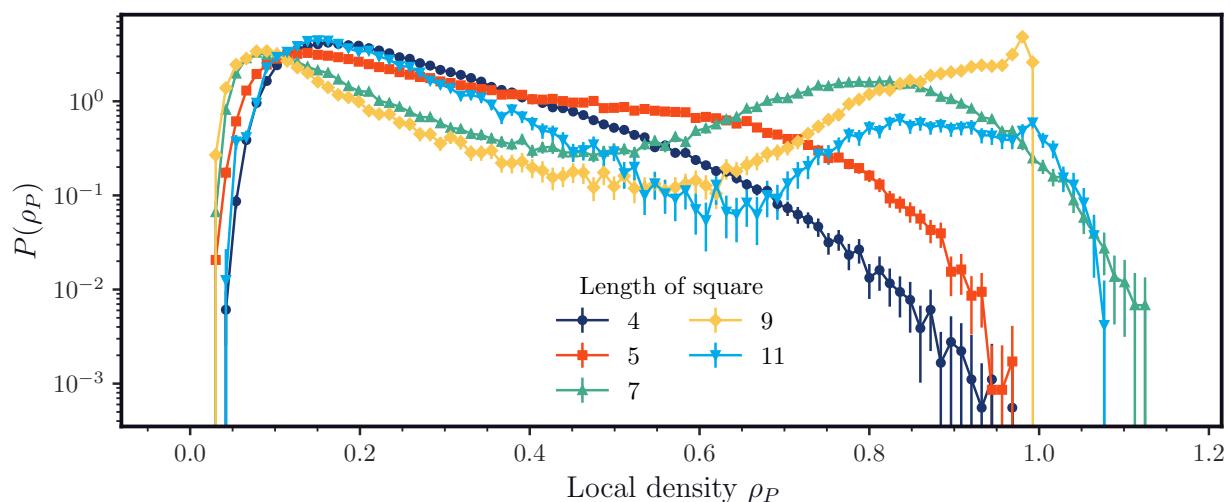


FIG. S1: Histograms of the local density of passive square particles of varying length for  $\phi_A = 0.2$ ,  $\phi_P = 0.2$ ,  $\nu = 80$ , and  $\omega = 5$ .

\* [rotskoff@stanford.edu](mailto:rotskoff@stanford.edu)

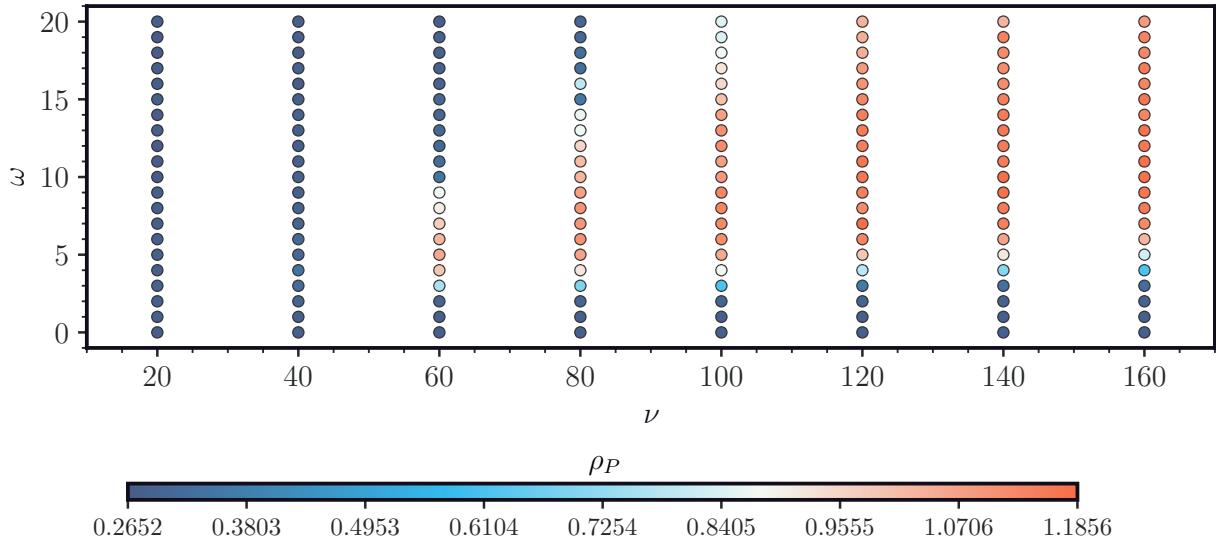


FIG. S2: Average density of passive square particles in the cluster phase for varying  $\nu$  and  $\omega$  for  $\phi_A = 0.2$ ,  $\phi_P = 0.2$ , and  $L = 9 \sigma$ . In cases where the system remains homogeneous, the cluster density is set equal to the overall passive particle density.

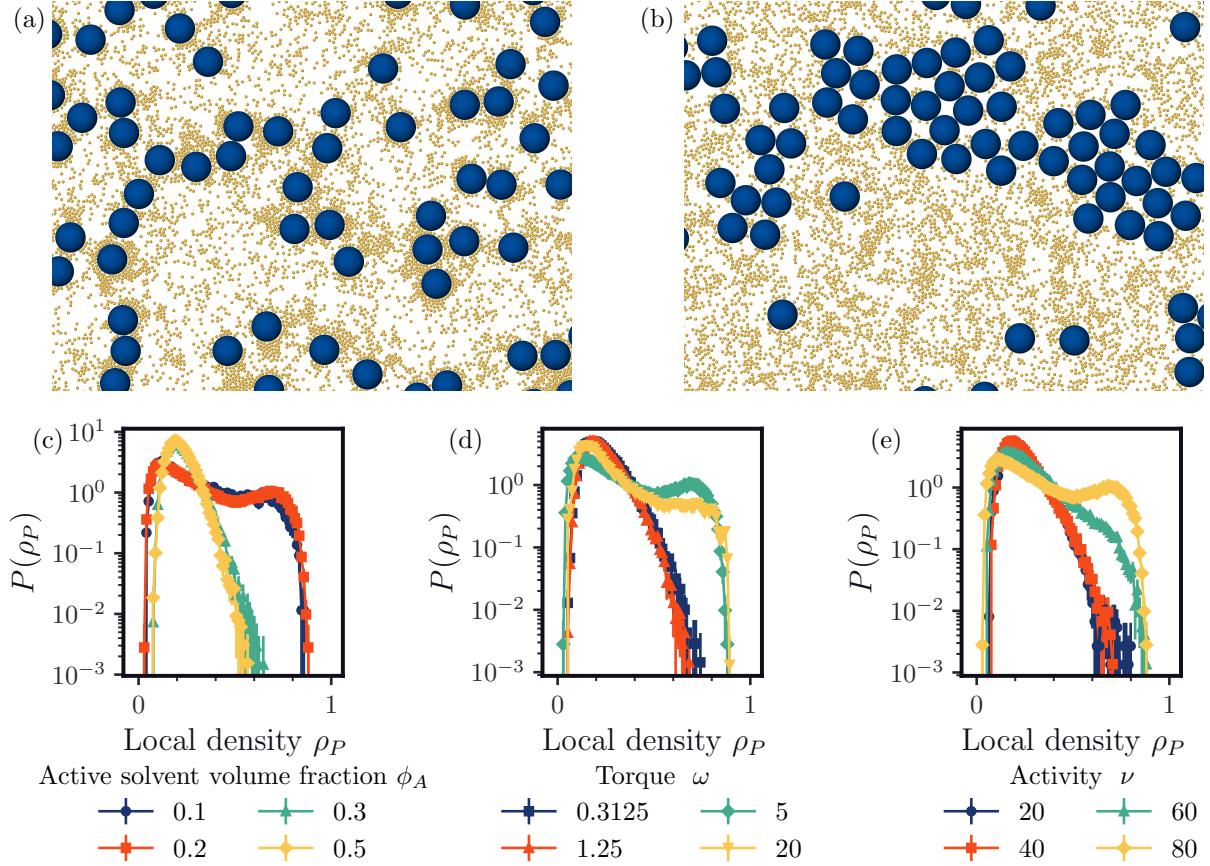


FIG. S3: Multiple passive disks of radii  $5\sigma$  in a chiral active Brownian particle bath with a passive volume fraction of 0.2. (a,b) Systems where the passive disks do not and do assemble for  $\phi_A = 0.2$ ,  $\nu = 80$ , and (a)  $\omega = 0.3125$  and (b)  $\omega = 5$ , respectively. Histograms of local density of the passive particles,  $\rho_P$ , for (c) varying  $\phi_A$  at  $\omega = 5$  and  $\nu = 80$ , (d) varying  $\omega$  at  $\phi_A = 0.2$  and  $\nu = 80$ , (e) varying  $\nu$  at  $\omega = 5$  and  $\phi_A = 0.2$ .

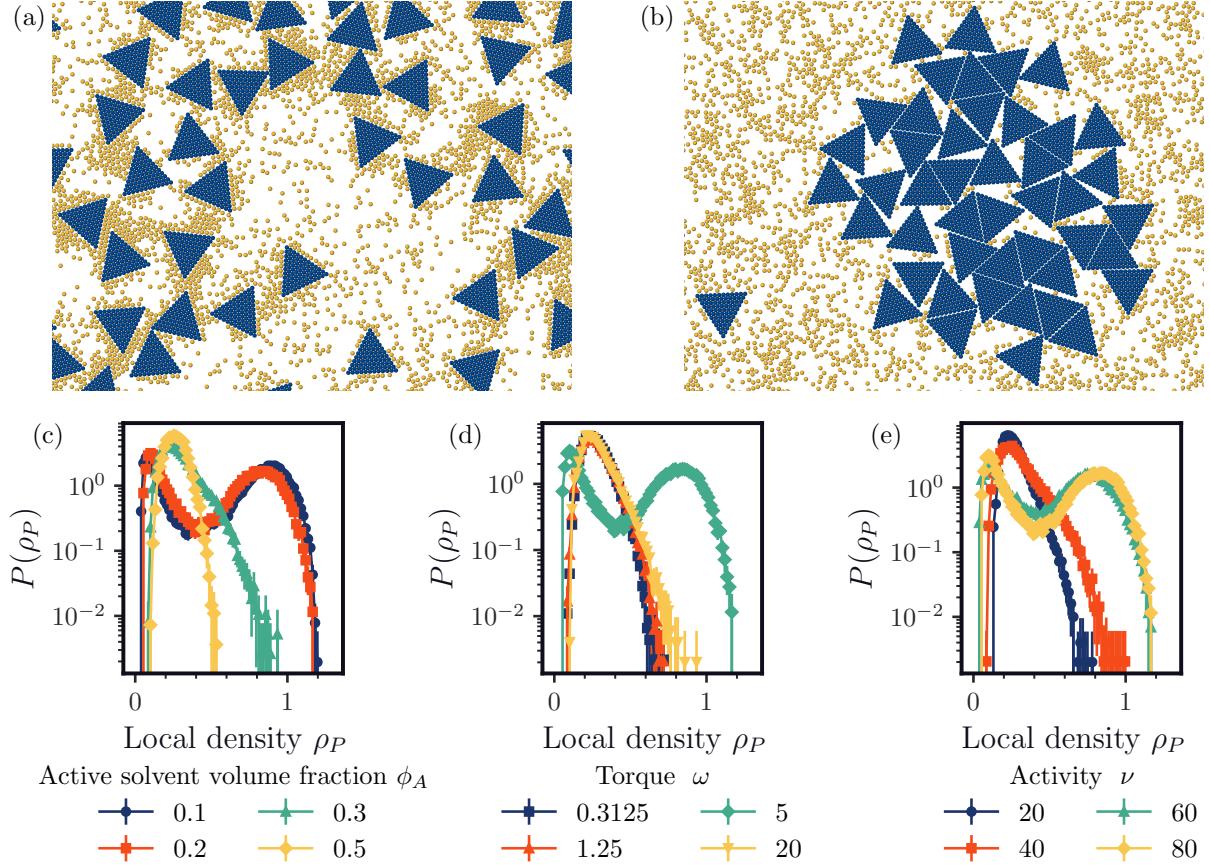


FIG. S4: Multiple passive triangles of side length  $12 \sigma$  in a chiral active Brownian particle bath with a passive volume fraction of 0.2. (a,b) Systems where the passive triangles do not and do assemble for  $\phi_A = 0.2$ ,  $\nu = 80$ , and (a)  $\omega = 0.3125$  and (b)  $\omega = 5$ , respectively. Histograms of local density of the passive particles,  $\rho_P$ , for (c) varying  $\phi_A$  at  $\omega = 5$  and  $\nu = 80$ , (d) varying  $\omega$  at  $\phi_A = 0.2$  and  $\nu = 80$ , (e) varying  $\nu$  at  $\omega = 5$  and  $\phi_A = 0.2$ .

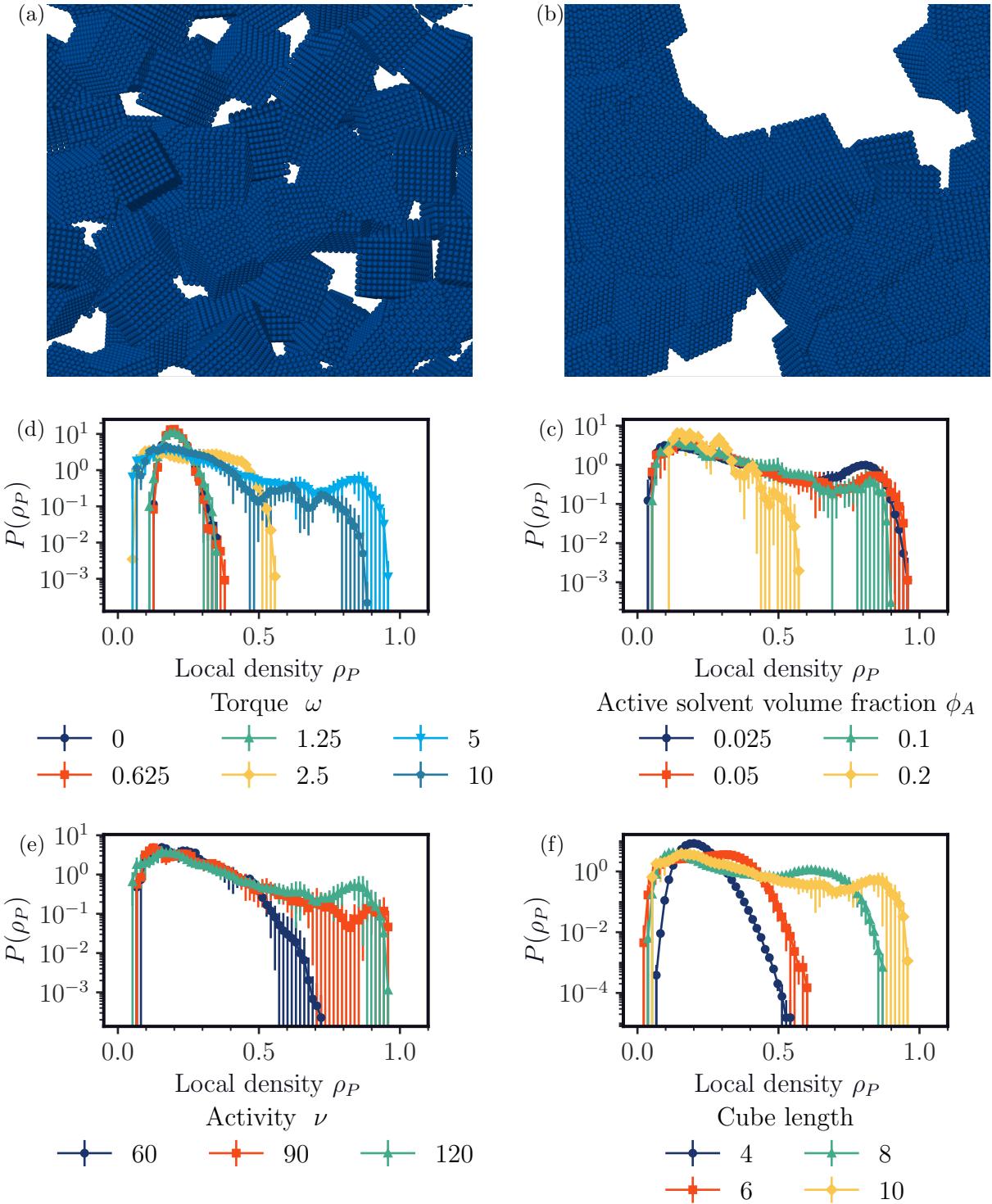


FIG. S5: Multiple passive cubes of length  $10\sigma$  in a chiral active Brownian particle bath with a passive volume fraction of 0.2 in three dimensions. (a,b) Systems where the passive cubes do not and do assemble for  $\phi_A = 0.2$ ,  $\nu = 120$ , and (a)  $\omega = 0.625$  and (b)  $\omega = 5$ , respectively, where the solvent is not visualized. Histograms of local density of the passive cube particles,  $\rho_P$ , for  $\phi_P = 0.2$  at (c) varying  $\omega$  with  $\phi_A = 0.05$ ,  $\nu = 120$  and  $L = 10\sigma$ , (d) varying  $\phi_A$  at  $\nu = 120$ ,  $\omega = 5$ , and  $L = 10\sigma$ , (e) varying  $\nu$  at  $\phi_A = 0.05$ ,  $\omega = 5$ , and  $L = 10\sigma$ , (f) varying  $L$  at  $\phi_A = 0.05$ ,  $\nu = 120$ , and  $\omega = 5$ .

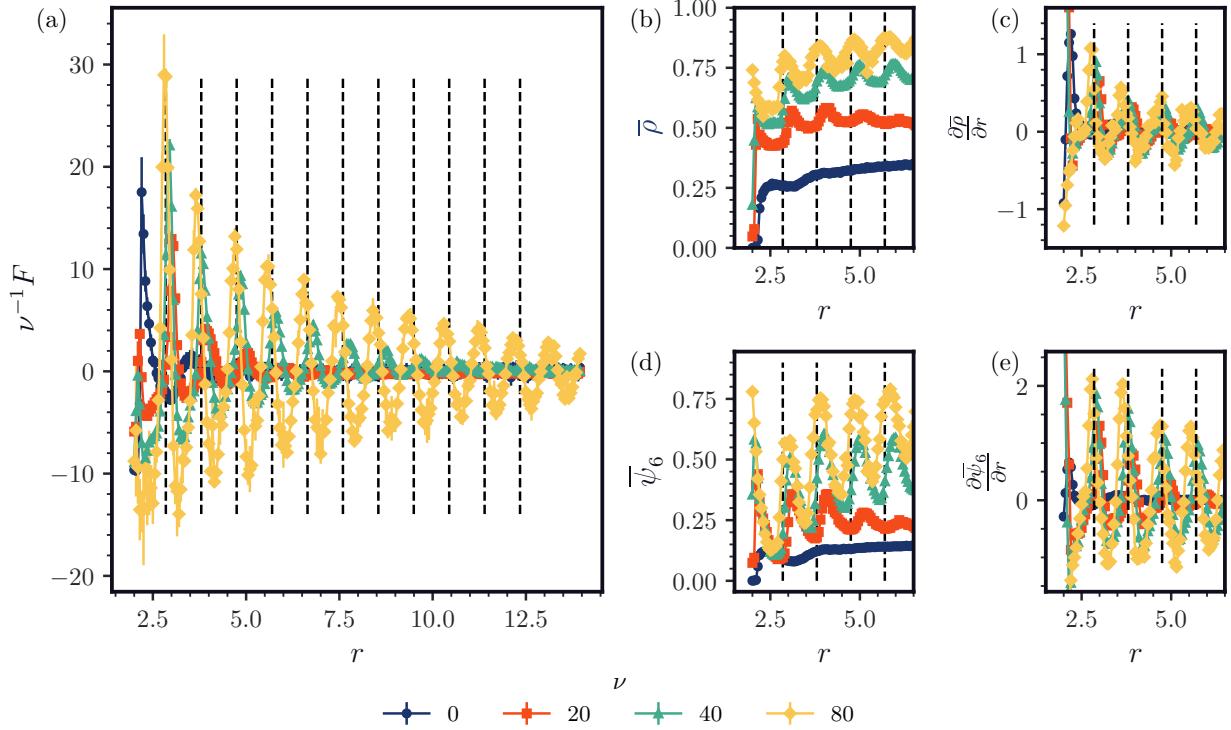


FIG. S6: Quantities obtained for a system with two passive walls of length 10 and  $\rho = 0.4$  for varying  $\nu$  and separation length. (a) Force  $F$ . (b) Density between walls,  $\bar{\rho}$ . (c) Hexatic order parameter between walls,  $\frac{\partial \bar{\rho}}{\partial r}$ . (d)  $\bar{\psi}_6$ . (e)  $\frac{\partial \bar{\psi}_6}{\partial r}$ . See Sec. C5 for further details on how the density and hexatic order parameter are computed.

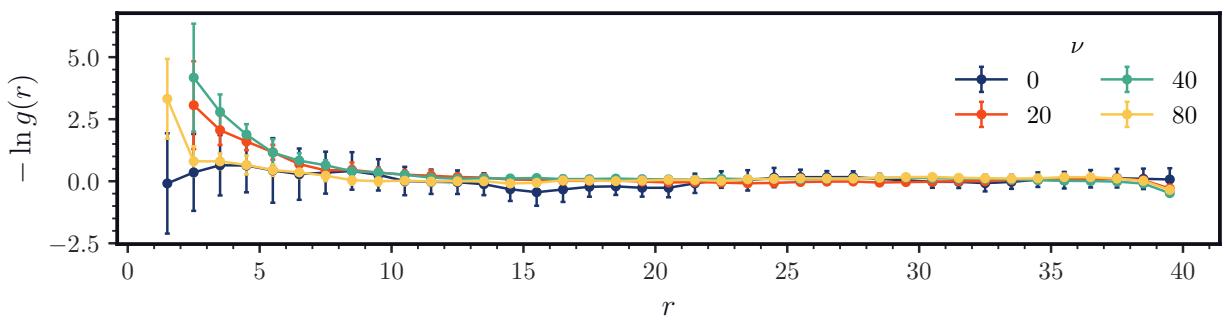


FIG. S7: The effective free energy  $-\ln g(r)$  between two passive walls of length 10 and  $\rho = 0.4$  for varying activity.

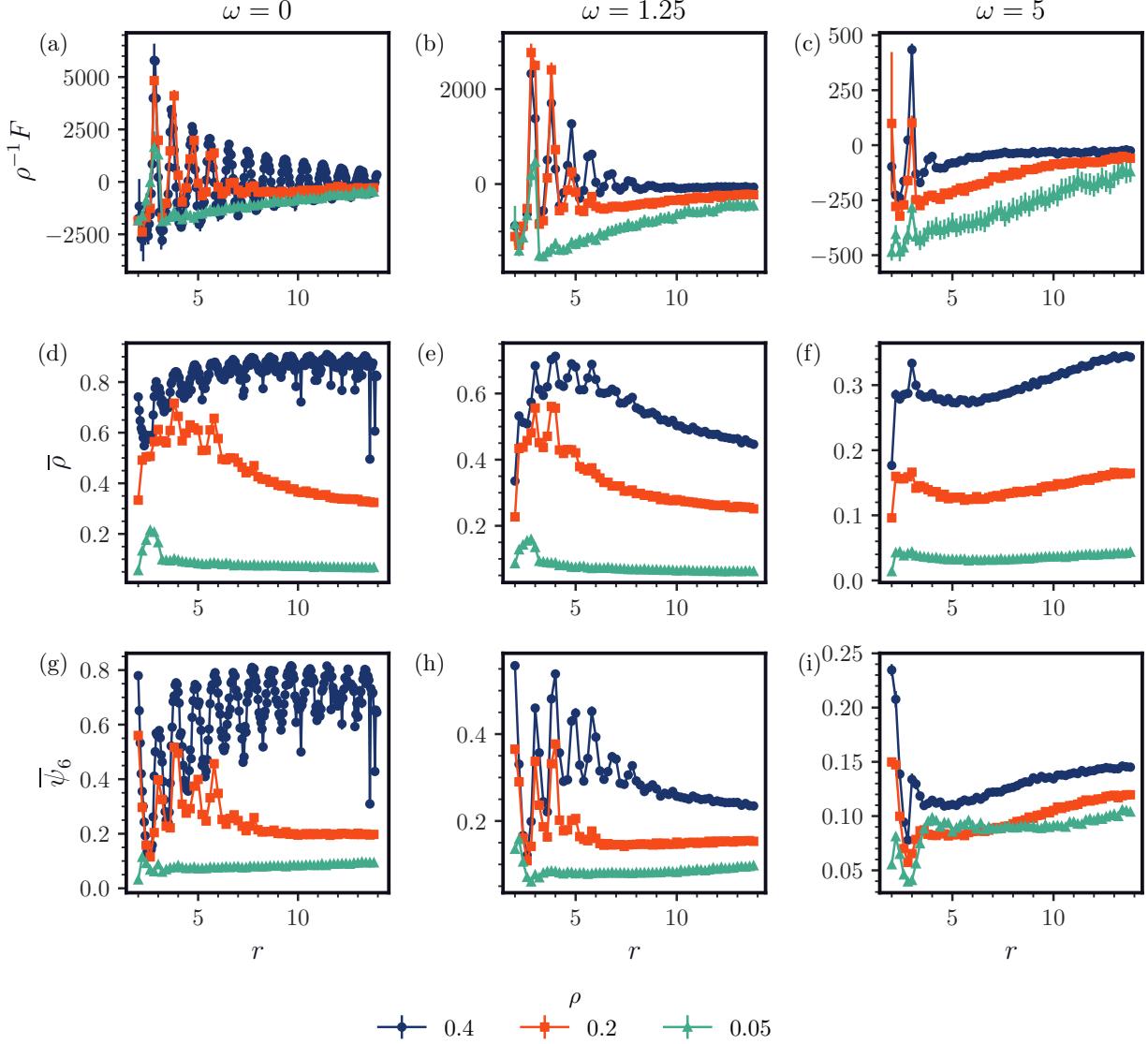


FIG. S8:  $\rho^{-1} F$ ,  $\bar{\rho}$ , and  $|\bar{\psi}_6|$  between two passive walls of length 10 for varying separation lengths, torque, and  $\rho$  for  $\nu = 80$ . See Sec. C5 for further details on how the density and hexatic order parameter are computed.

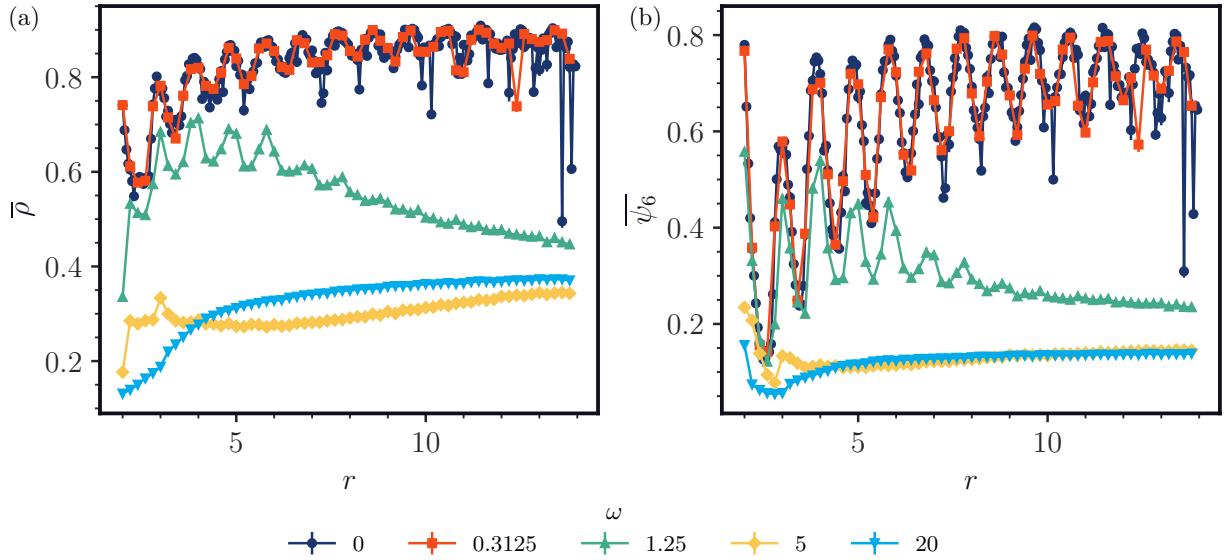


FIG. S9: (a) Average density  $\bar{\rho}$  and (b) hexatic order parameter  $|\bar{\psi}_6|$  between two passive walls of length 10, bulk  $\rho = 0.4$ , and  $\nu = 80$  for varying torque and separation length. See Sec. C5 for further details on how the density and hexatic order parameter are computed.

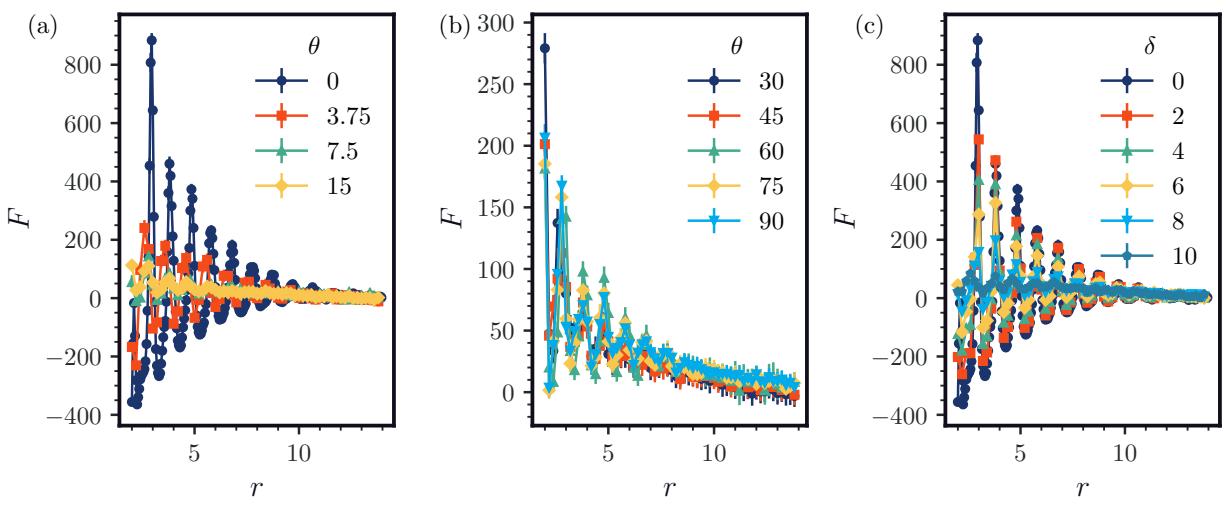


FIG. S10: Force between two passive walls of length 10,  $\rho = 0.4$ , and  $\nu = 40$  for (a,b) varying angles  $\theta$  between the walls and (c) varying offset  $\delta$  between the walls.

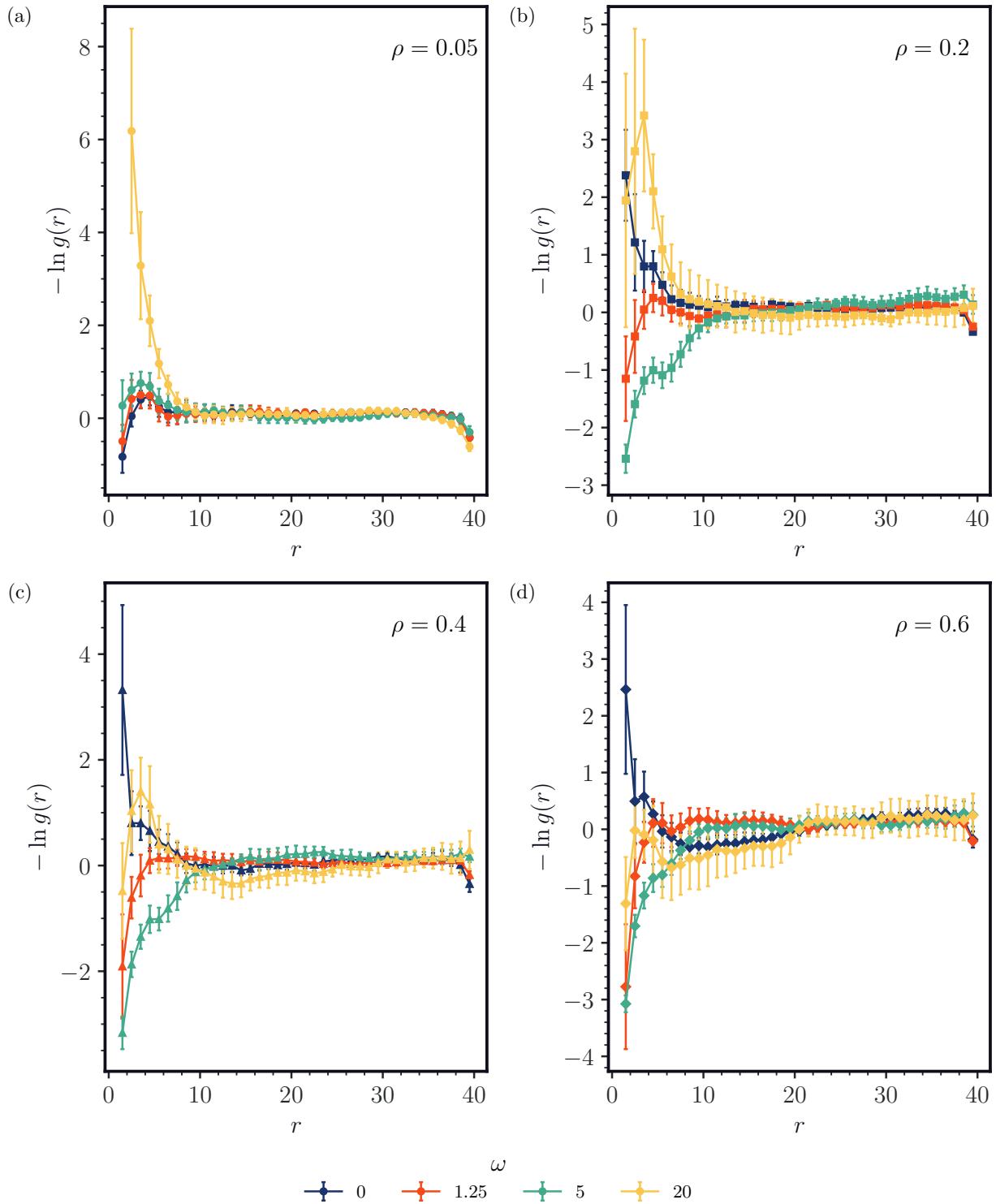


FIG. S11: Effective free energy between two passive walls of length 10 and  $\nu = 80$  for varying  $\rho$  and  $\omega$ .

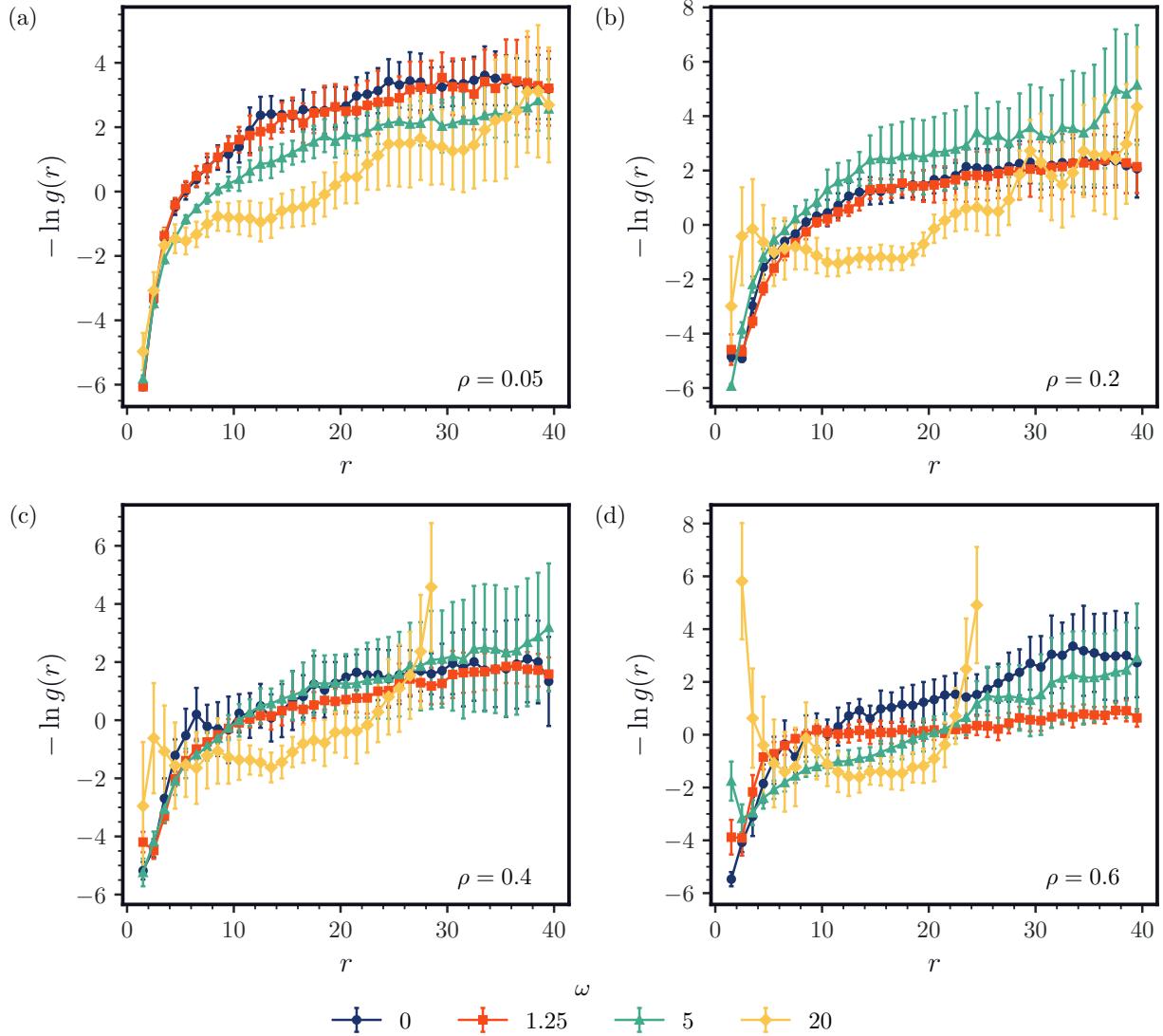


FIG. S12: Effective free energy between two passive walls of length 10 and  $\nu = 80$  for varying  $\rho$  and  $\omega$  that are constrained to move only in the  $x$ -direction and to not rotate. See Sec. C6 for further details on how the constraint is implemented.

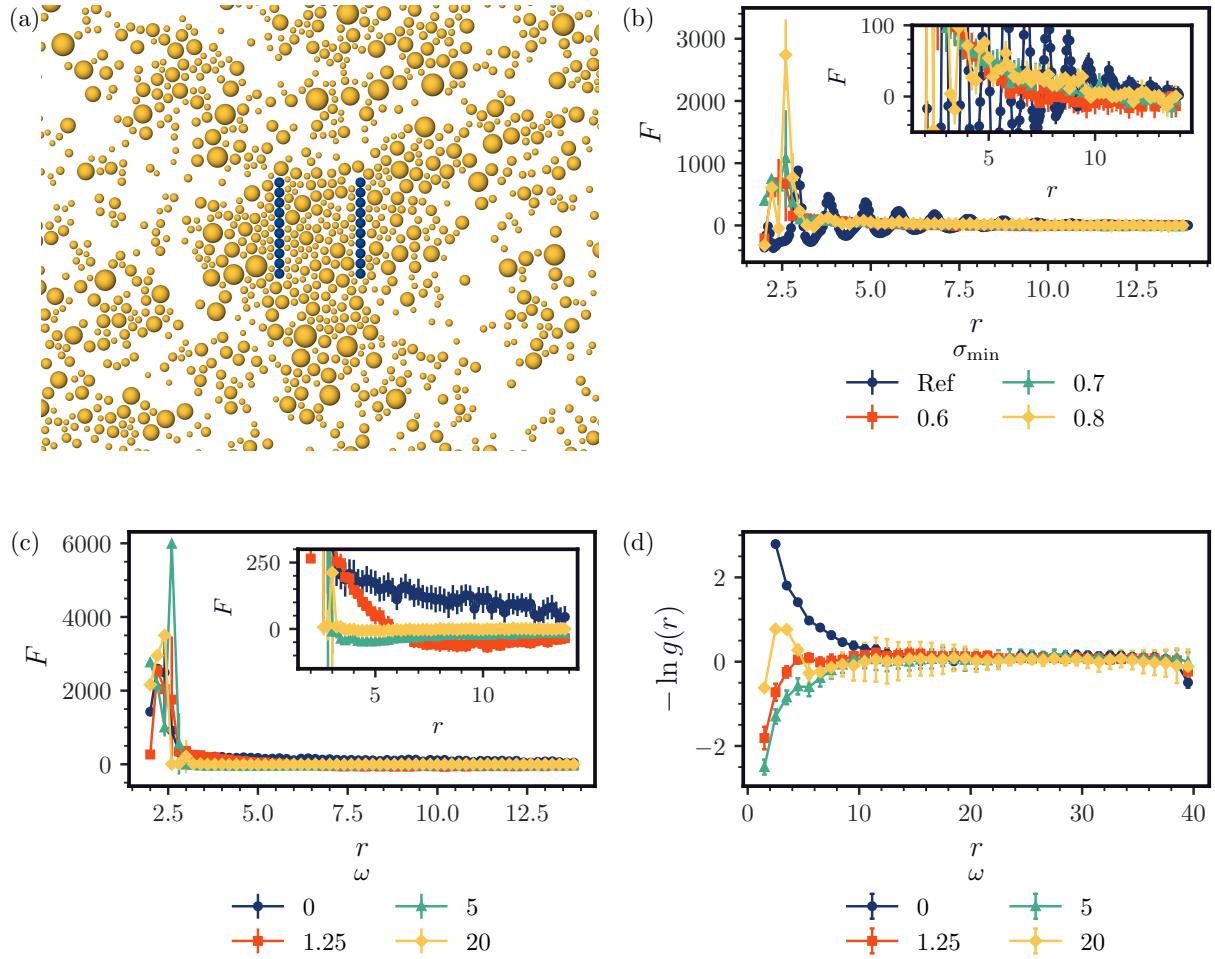
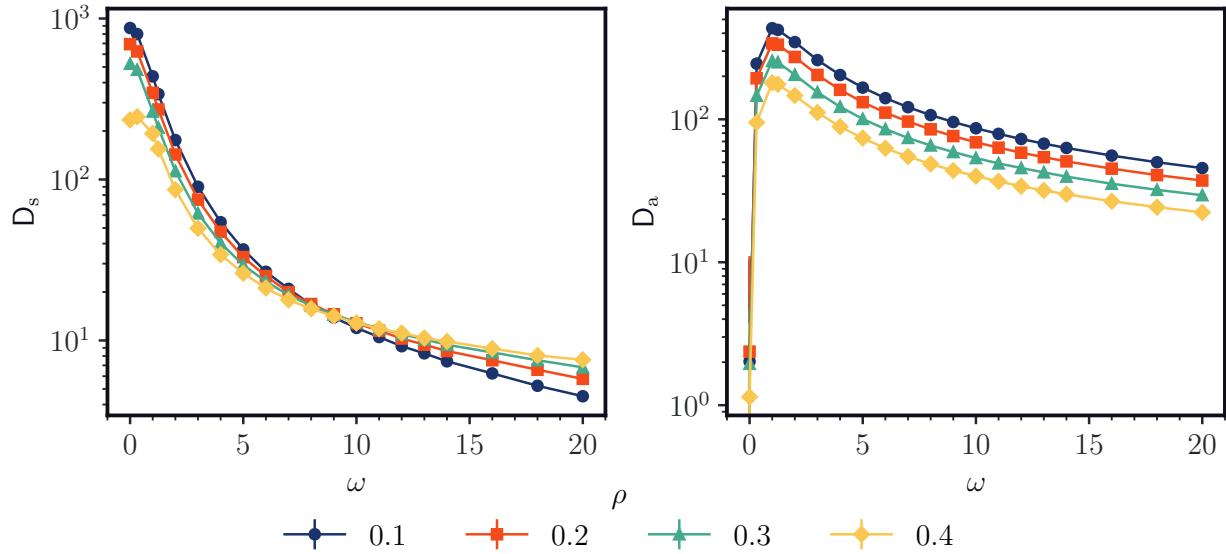
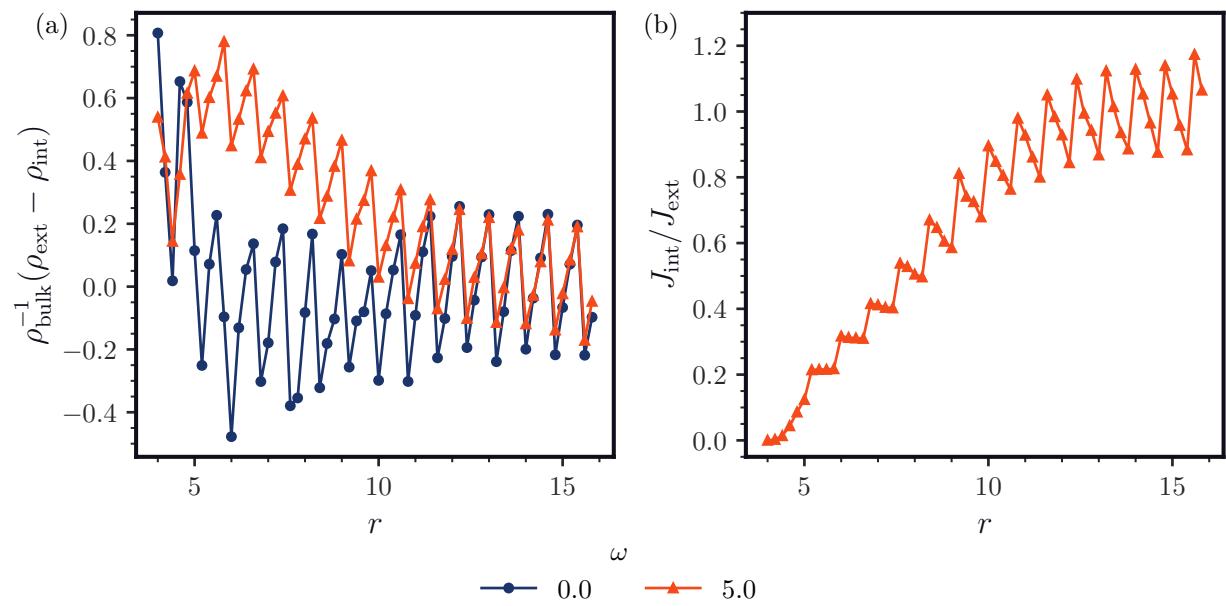


FIG. S13: Passive walls in a polydisperse active Brownian particle bath system. (a) Image of the system with  $\rho = 0.4$ ,  $\nu = 40$ , and  $\sigma_{\min} = 0.6$ . (b) Force between two passive walls of length 10,  $\rho = 0.4$ ,  $\nu = 40$ , and  $\omega = 0$  for varying separation lengths and  $\sigma_{\min}$ . (c) Force and (d)  $-\ln g(r)$  between two passive walls of length 10,  $\rho = 0.4$ ,  $\nu = 80$ , and  $\sigma_{\min} = 0.6$  for varying separation lengths and  $\omega$ .

FIG. S14: Diffusion constants for varying  $\omega$  and  $\rho$  at  $\nu = 80$ .FIG. S15: (a) Difference between external and internal densities and (b) ratio of internal and external fluxes near the walls for varying  $\omega$  at  $\nu = 80$  and  $\rho = 0.2$ .

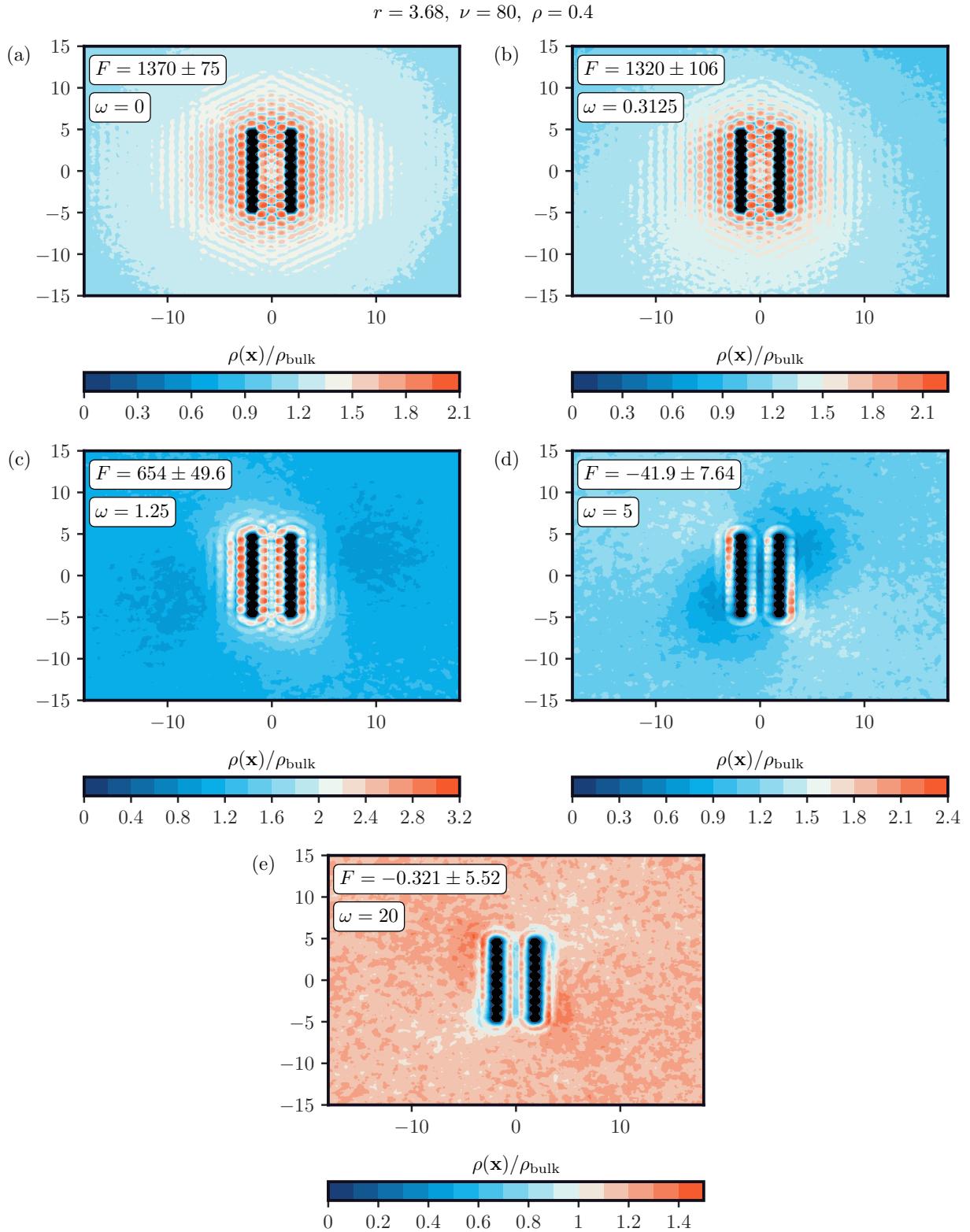


FIG. S16: Density fields for maximal repulsive force between two passive walls in a chiral active Brownian particle bath.

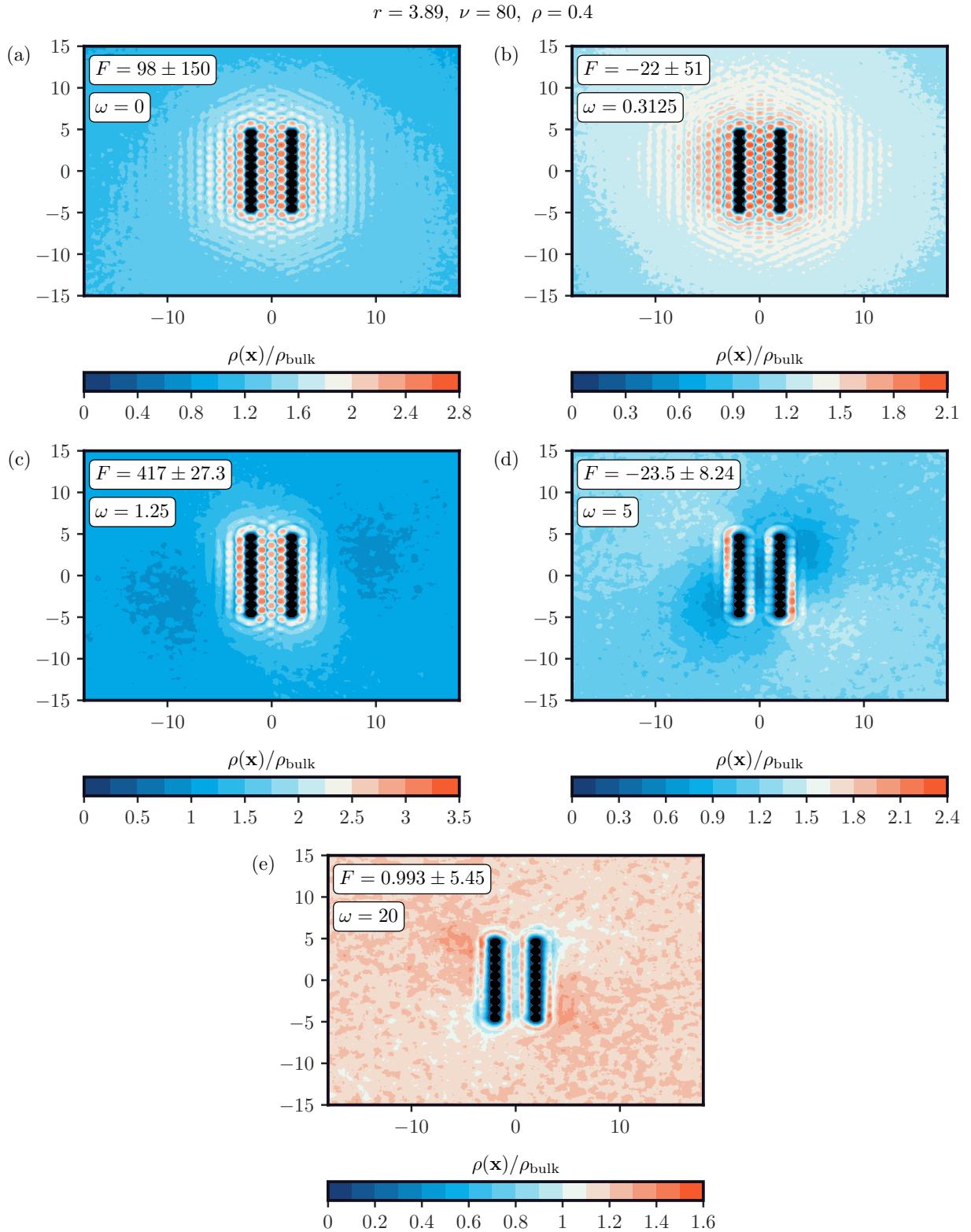


FIG. S17: Density fields for a separation with near zero force between two passive walls in a chiral active Brownian particle bath.

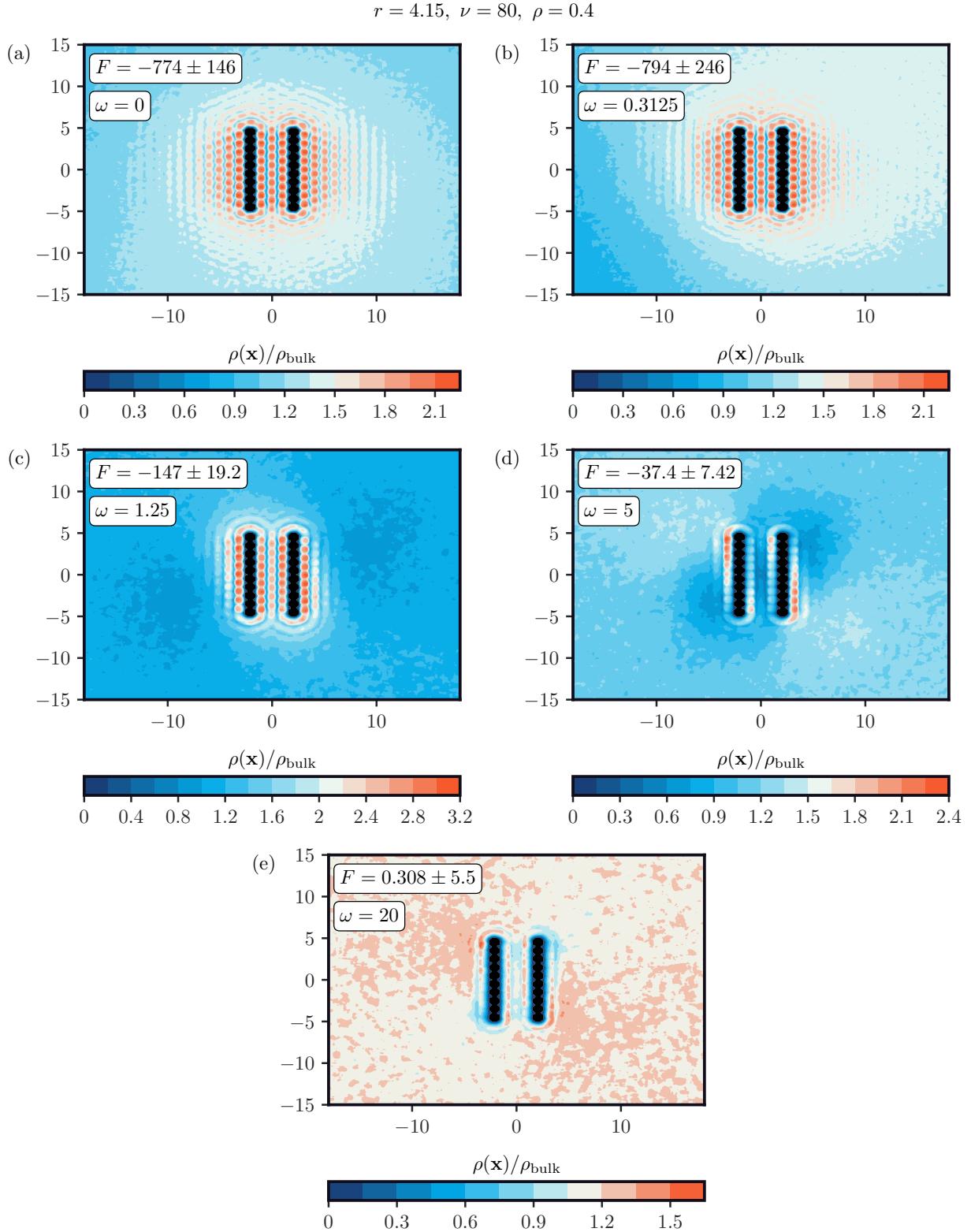


FIG. S18: Density fields for maximal attractive force between two passive walls in a chiral active Brownian particle bath.

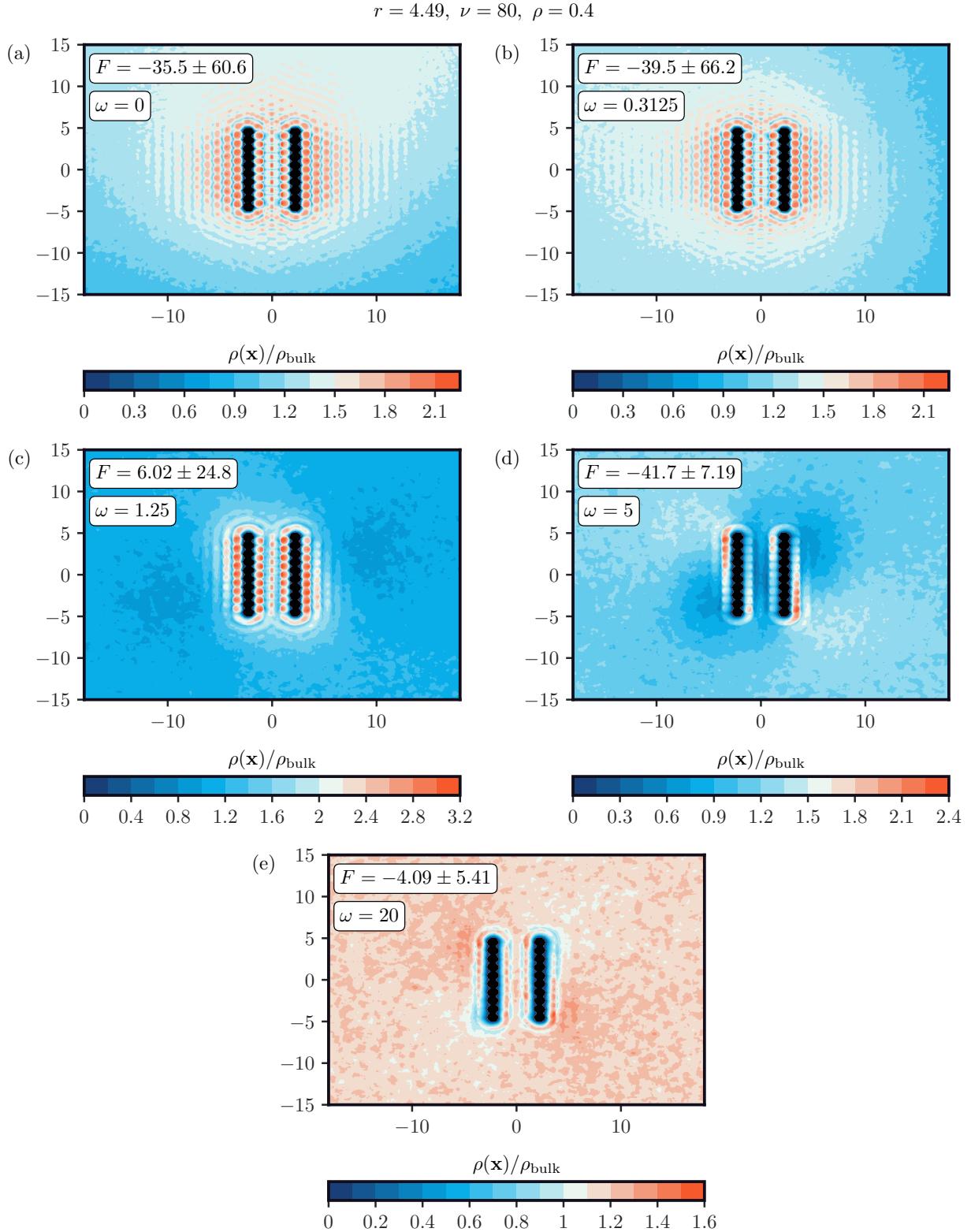


FIG. S19: Density fields for a separation with near zero force between two passive walls in a chiral active Brownian particle bath.

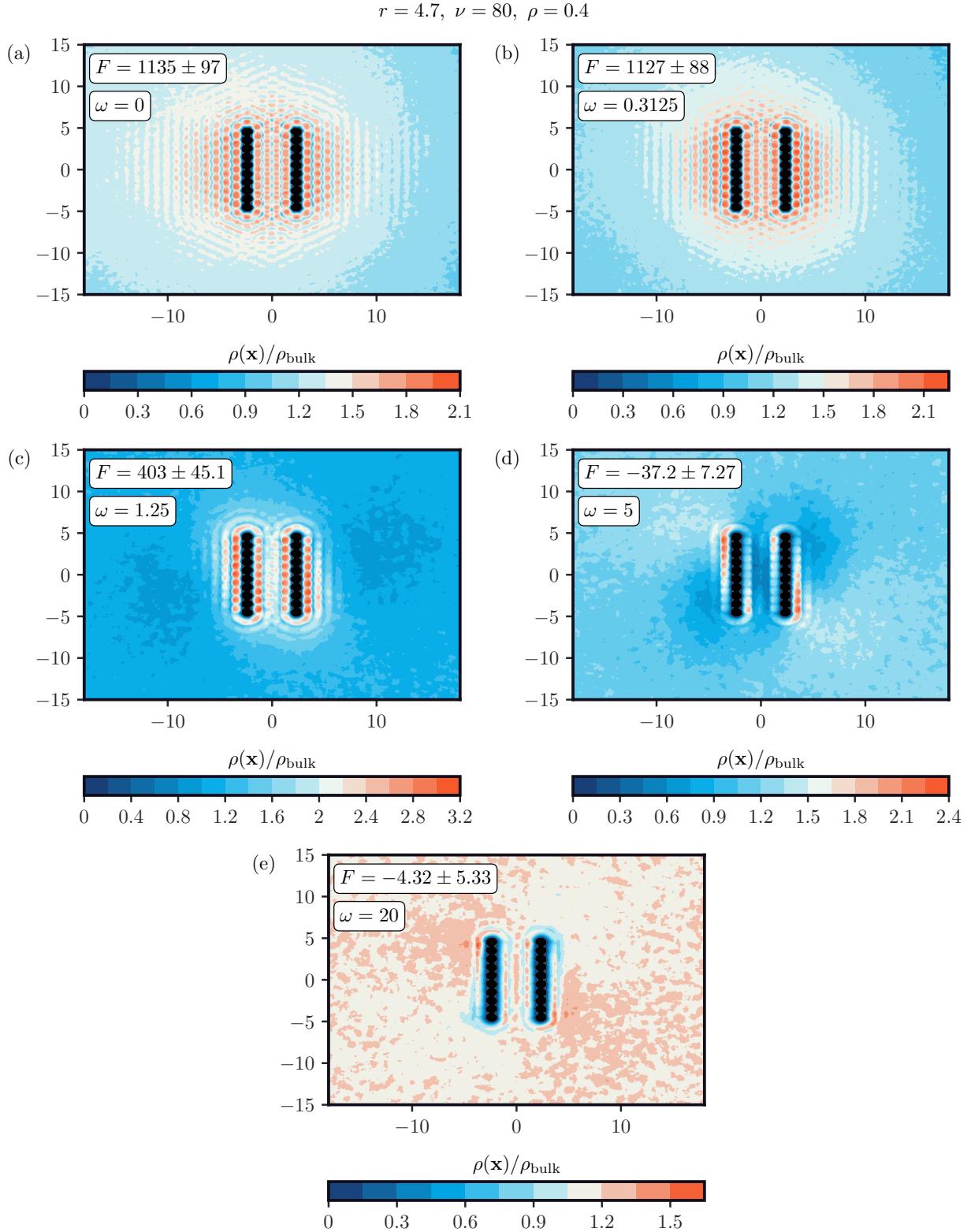


FIG. S20: Density fields for maximal repulsive force between two passive walls in a chiral active Brownian particle bath.

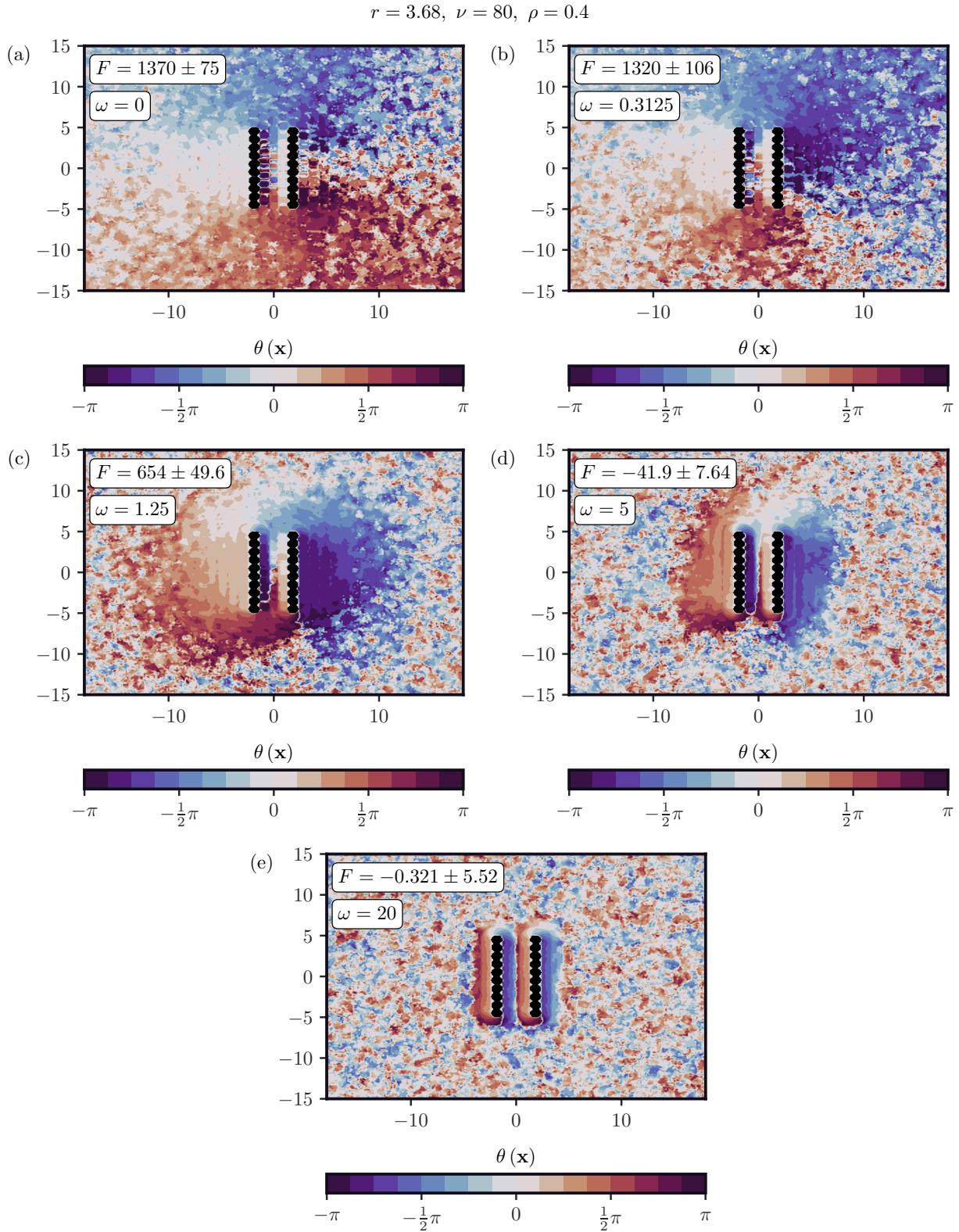


FIG. S21: Orientation fields for maximal repulsive force between two passive walls in a chiral active Brownian particle bath.

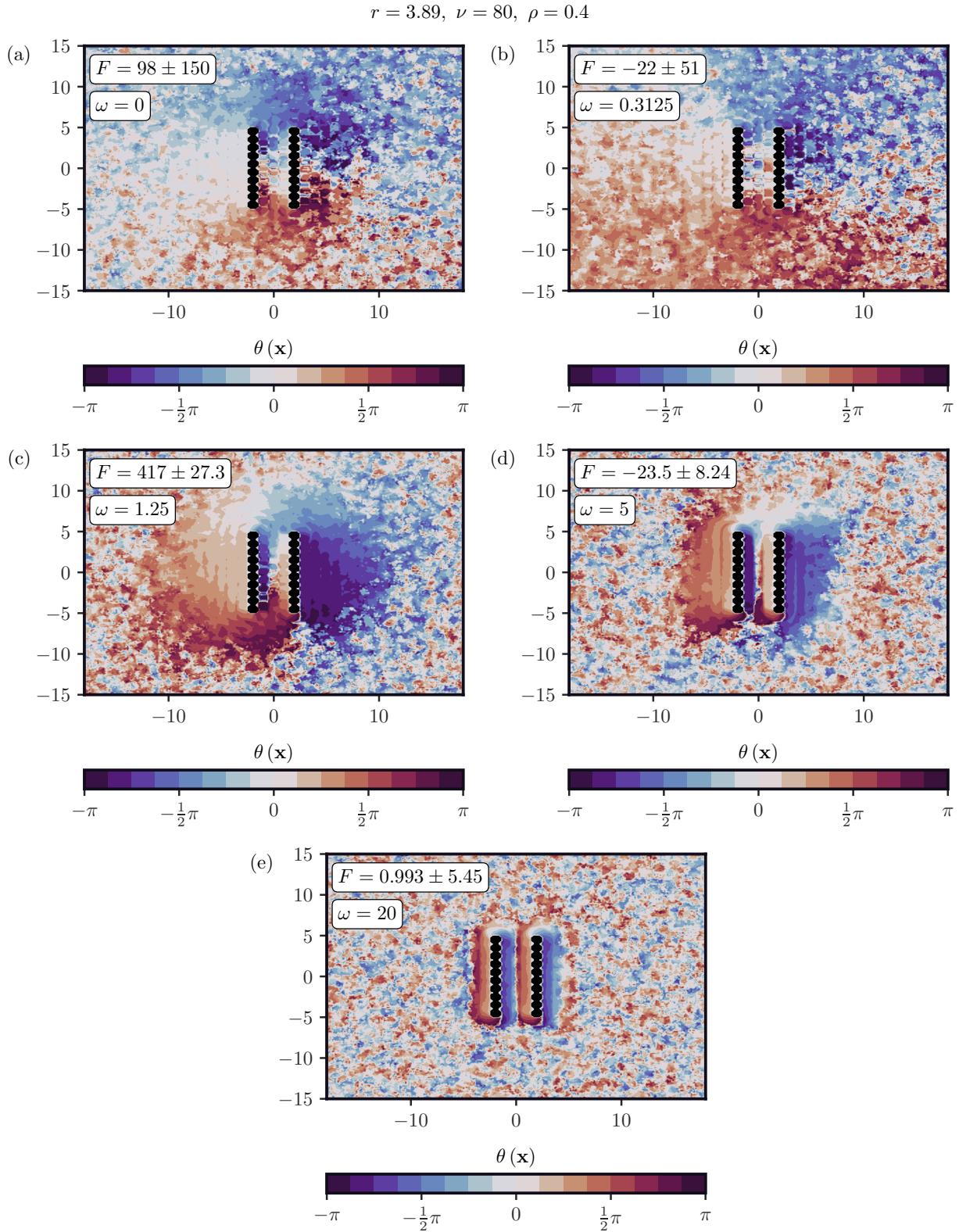


FIG. S22: Orientation fields for a separation with near zero force between two passive walls in a chiral active Brownian particle bath.

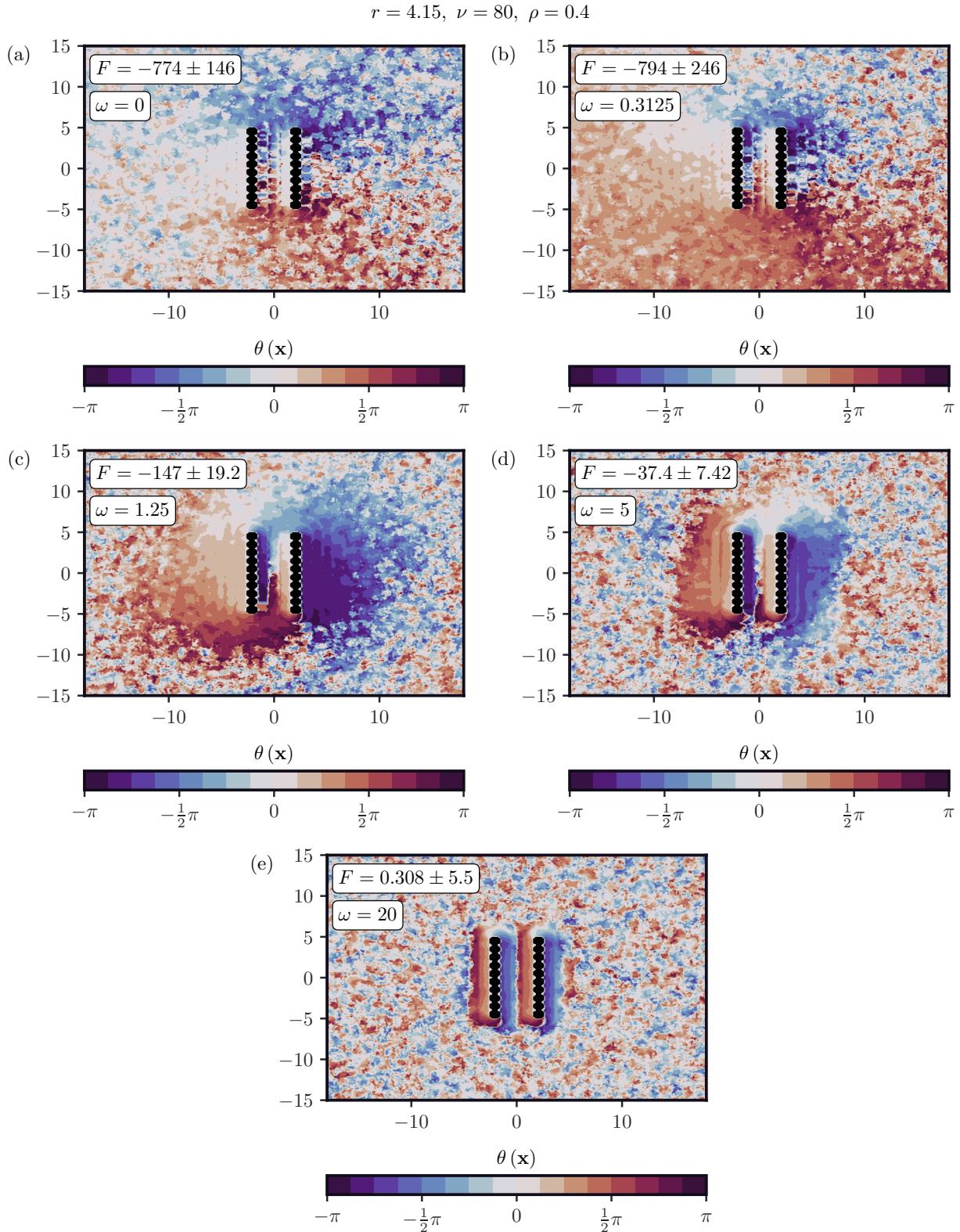


FIG. S23: Orientation fields for maximal attractive force between two passive walls in a chiral active Brownian particle bath.

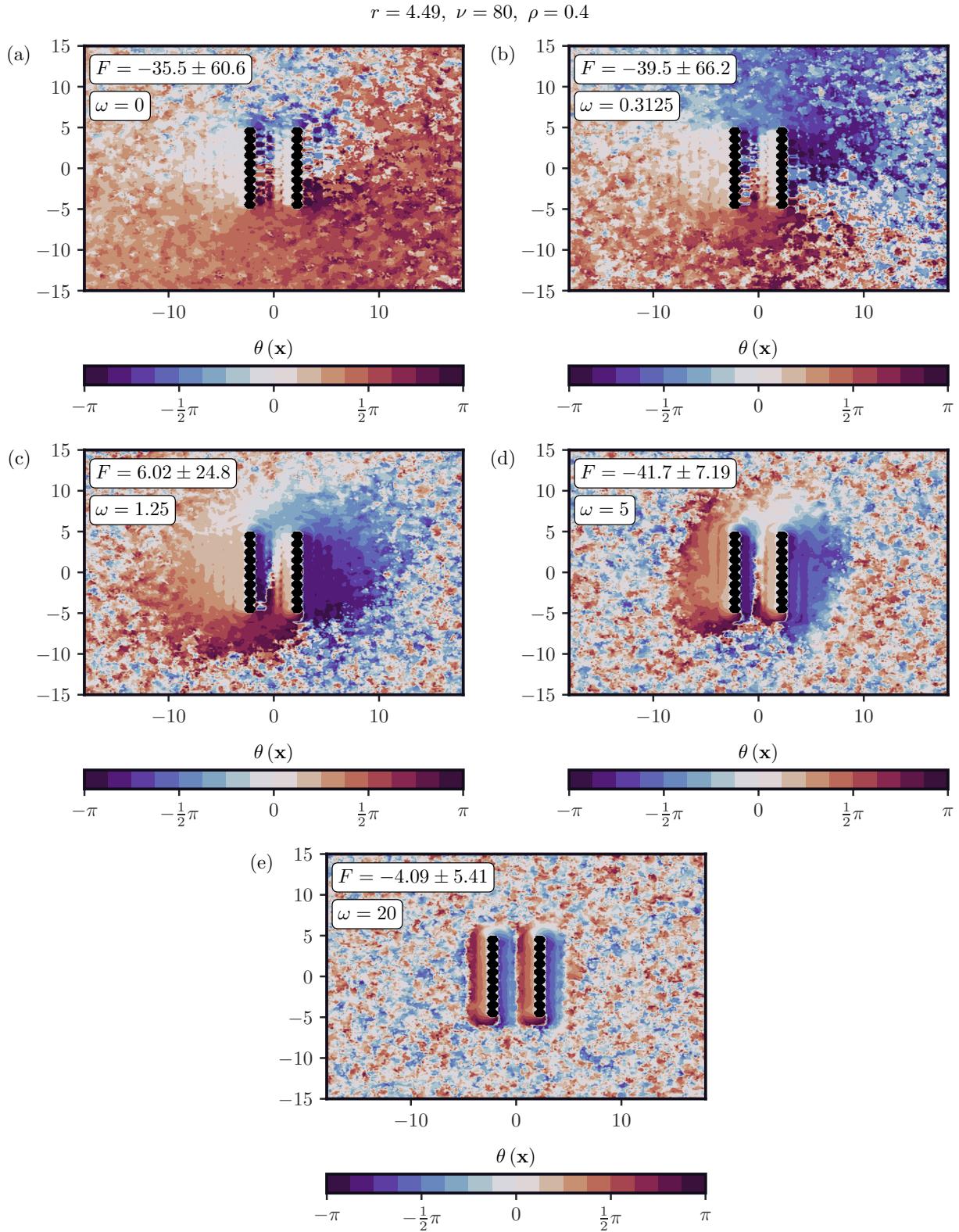


FIG. S24: Orientation fields for a separation with near zero force between two passive walls in a chiral active Brownian particle bath.

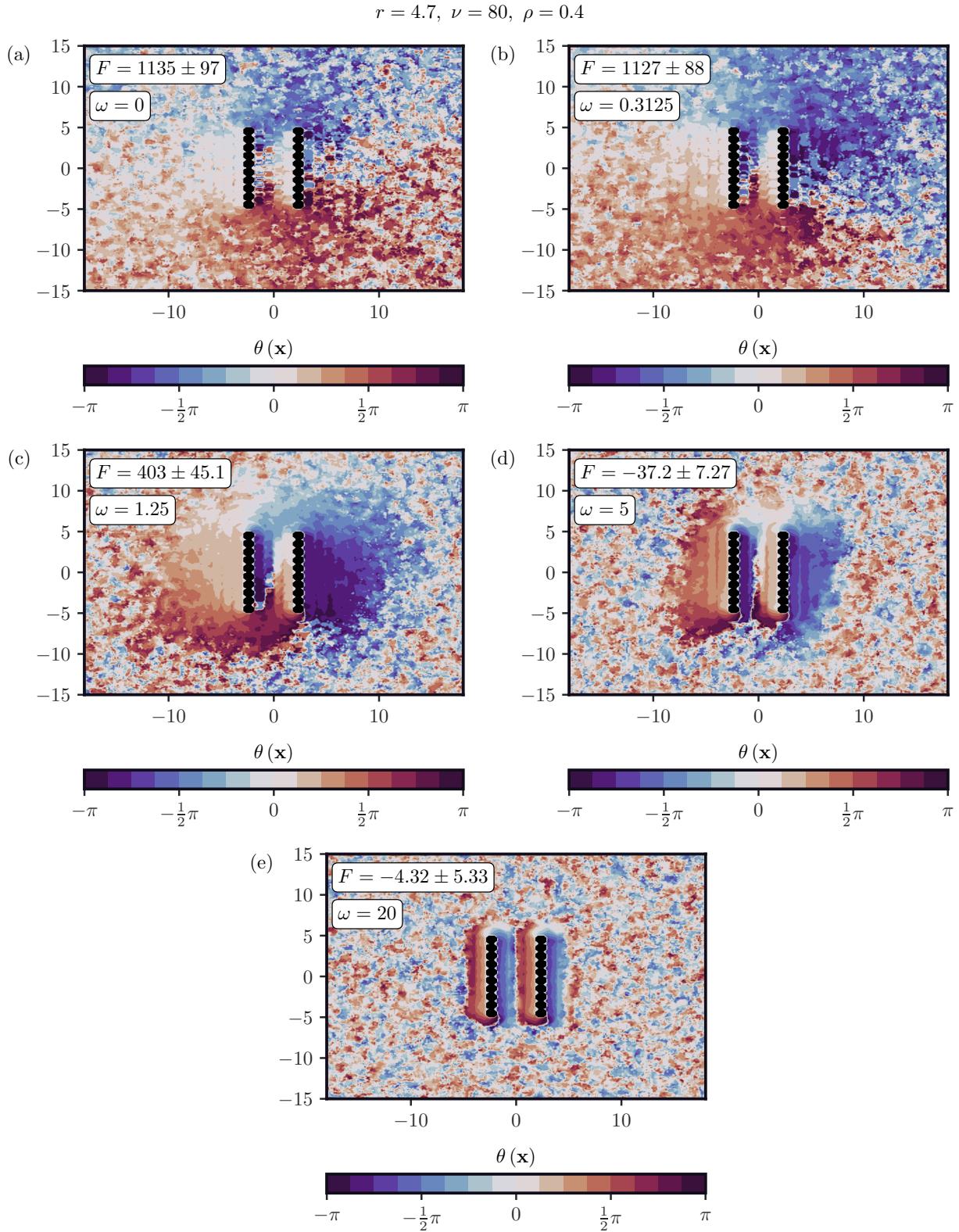


FIG. S25: Orientation fields for maximal repulsive force between two passive walls in a chiral active Brownian particle bath.