1 Varying External Potential

We consider the overdamped DDFT with no flux boundary conditions, a Gaussian pair potential and for the forward problem, no background flow. The external potential is given by

$$V_{ext} = \cos(2\pi(t + 0.5)/2.75)r^2,$$

see Figure 1. The time horizon for the problem is $(0, 3)$ with $n = 30$ and the spatial domain is a box of dimension $[-5, 5]^2$ with $N = 30$. The initial condition for ρ is the uniform distribution $\rho_0 = 0.8$. The ODE tolerances are set to be 10^{-8}. All figures show the time points 2, 5, 8, 10, 12, 14, 16, 18, 20, 23, 26 out of 30. While Figure 2 shows the effect of V_{ext} in absence of the interaction term, Figures 3 and 4 show the effect of the positive and negative attraction term in absence of the external potential. We note that the change in ρ by these interactions is of the same magnitude as the effect of V_{ext}. In Figures 5 and 6 the effects of V_{ext} in combination with the two different interaction potentials are shown. Note that in Figure 5 the maximum of the colour range is $\max \rho - 1.2$ in order to capture all important aspects of the dynamics over the time horizon. All other plots show the colour range $(\min \rho, \max \rho)$.

These forward problems are now used in the context of an optimal control problem. We are interested in optimizing a system without external potential present to mimic those with the chosen external potential. Therefore, we first set $\widehat{\rho}$ to be the forward problem without particle interactions ($\kappa = 0$) and with the external potential, see Figure 2. We then start the optimization by choosing the same uniform initial condition for ρ but without an external potential. The intitial guess for $\mathbf{w}$ is zero. We then expect $\mathbf{w}$ to mimic the external potential, forcing particles in the desired state and it is of interest in what way this flow control is similar to the external potential that shaped $\widehat{\rho}$. The same experiment is conducted with repulsive particles ($\kappa = 0.5$), where Figure 5 shows the desired state and Figure 3 displays the uncontrolled, initial state for the optimization. Then for attractive particles ($\kappa = -0.$) we have that $\widehat{\rho}$ takes the form shown in Figure 6, while the uncontrolled profile of ρ is displayed in Figure 4.

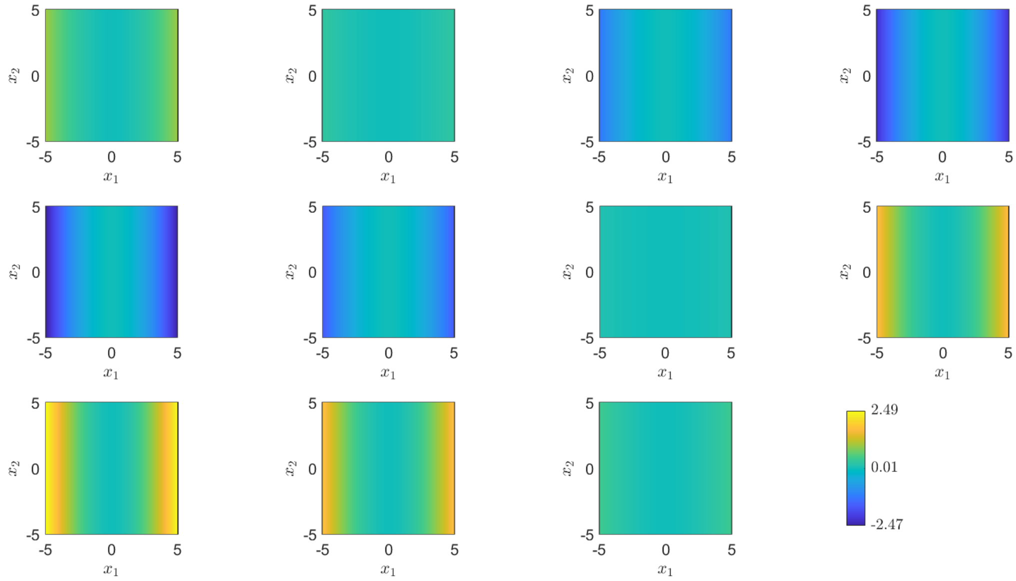

Figure 1: External potential over time.

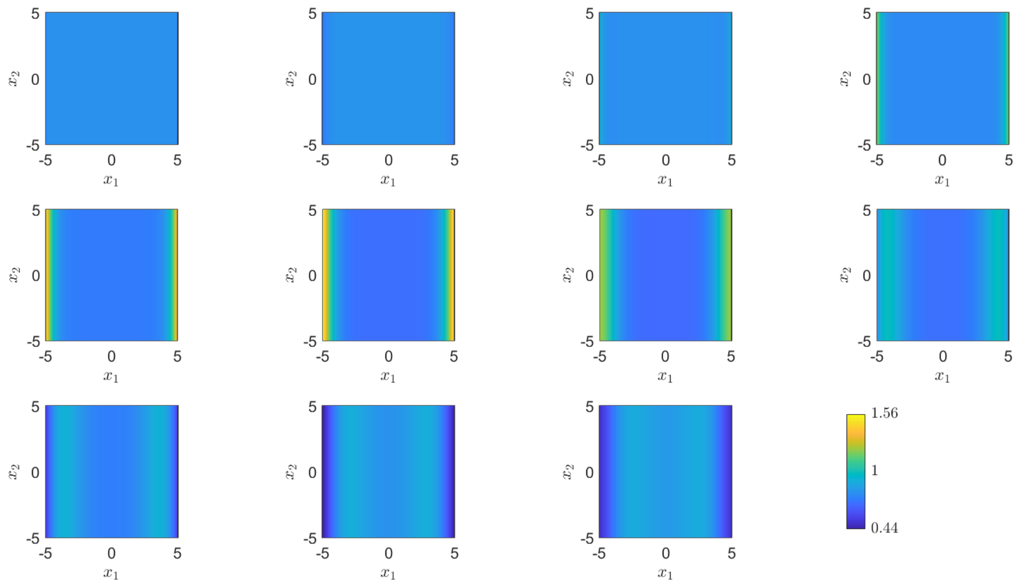

Figure 2: Forward ρ over time horizon, $\kappa = 0$, V_{ext} on. This is the desired state $\widehat{\rho}$ for the uncontrolled particle distribution without interactions, which is a uniform distribution.

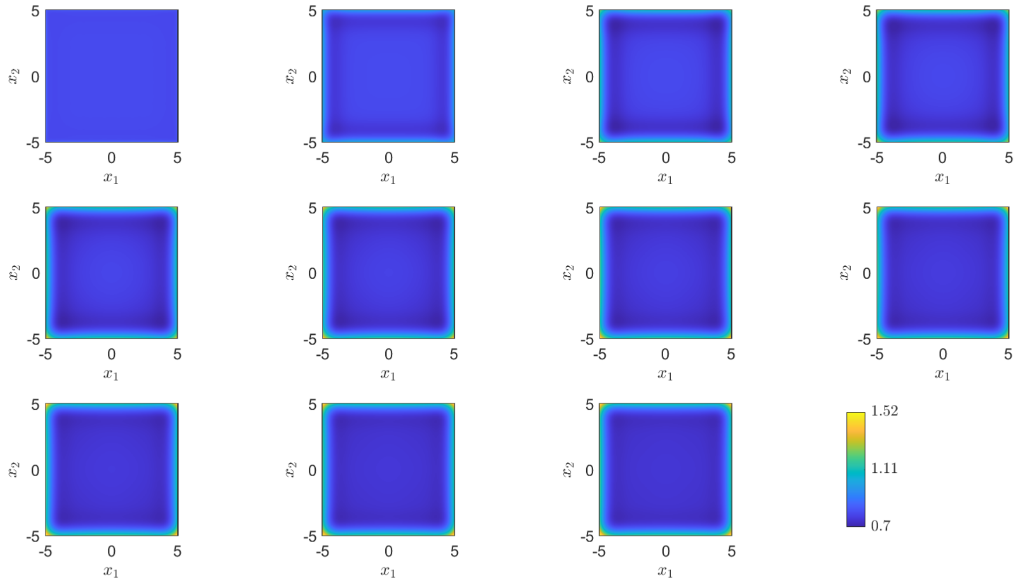

Figure 3: Forward ρ over time horizon, $\kappa = 0.5$, V_{ext} off. This is the uncontrolled state corresponding to the desired state $\widehat{\rho}$ displayed in Figure 5.

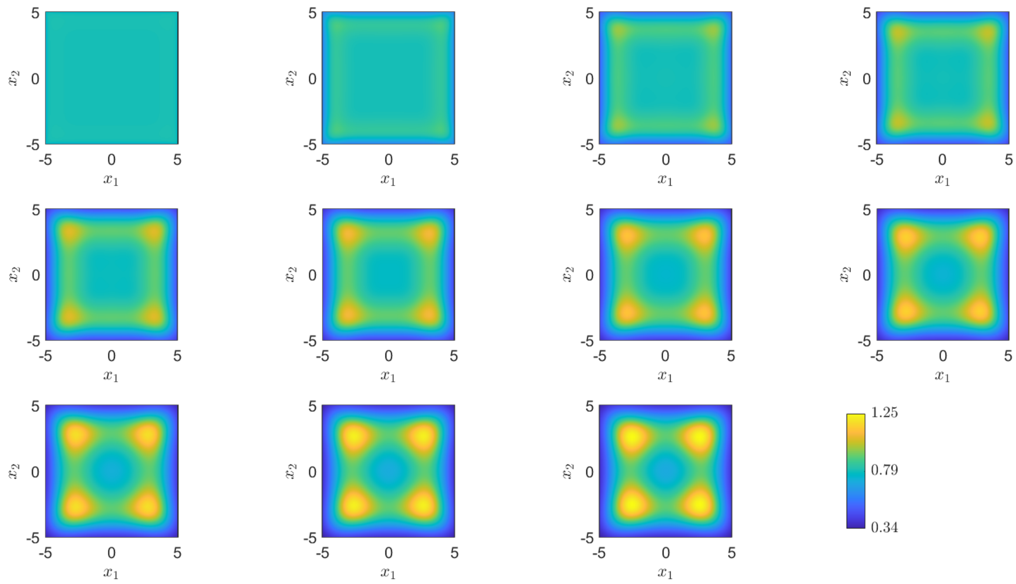

Figure 4: Forward ρ over time horizon, $\kappa = -0.5$, V_{ext} off. This is the uncontrolled state corresponding to the desired state $\widehat{\rho}$ displayed in Figure 6.

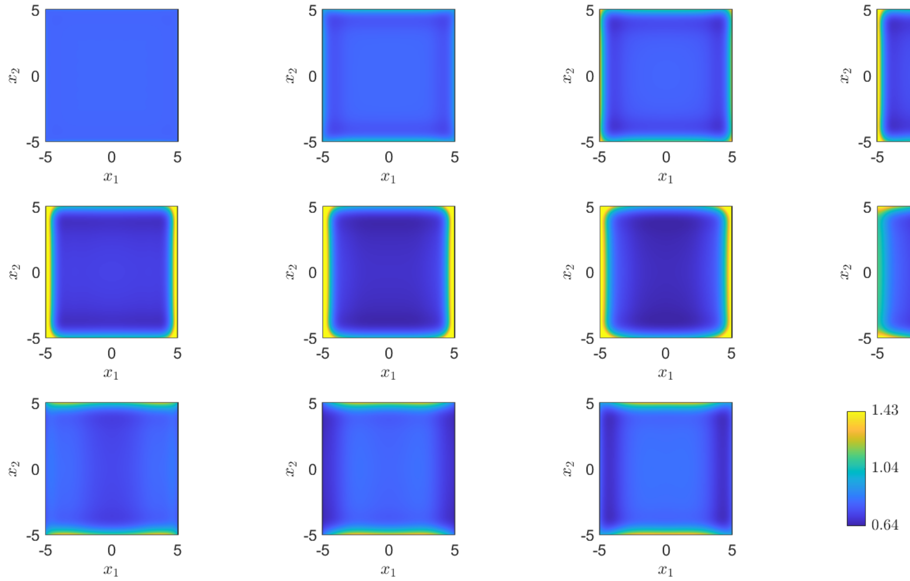

Figure 5: Forward ρ over time horizon, $\kappa = 0.5$, V_{ext} on. Note that the colour range is from $\min \rho$ to $(\max \rho) - 1.2$ for illustratory purposes. This is the desired state $\widehat{\rho}$ for the uncontrolled particle distribution shown in Figure 3.

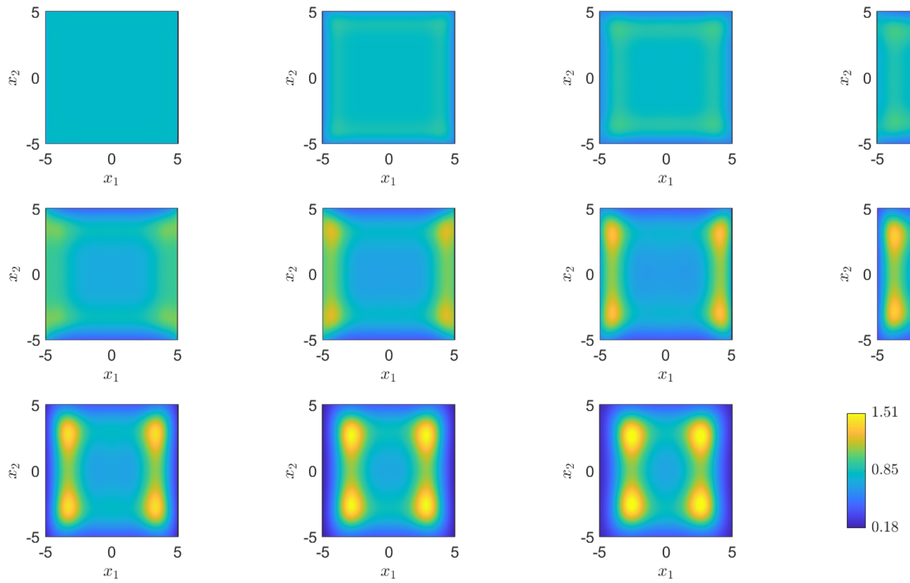

Figure 6: Forward ρ over time horizon, $\kappa = -0.5$, V_{ext} on. This is the desired state $\widehat{\rho}$ for the uncontrolled particle distribution shown in Figure 4.