1. Apply generic mean-field decoupling to $b_i^\dagger b_j$:

$$b_i^\dagger b_j \approx b_i^\dagger \langle b_j \rangle + \langle b_i^\dagger \rangle b_j - \cancel{\langle b_i^\dagger \rangle \langle b_j \rangle}$$

constant (neglected in the following)

Then, $$-J \sum_{\langle i,j \rangle} b_i^\dagger b_j \approx \sum_j \Big[-J \Big[b_j^\dagger \Big(\sum_{i \text{ NN of } j} \langle b_i \rangle \Big) + \Big(\sum_{i \text{ NN } j} \langle b_i^\dagger \rangle b_j \Big) \Big] =: \sum_j H_j^0 \left(\{\langle b_i \rangle\}, \{\langle b_i^\dagger \rangle\} \right)$$

i.e. $$H \approx \sum_j \left(H_j^0 + \frac{U}{2} n_j (n_j - 1) \right) =: \sum_j H_j$$

2. (i) Replace $\langle b_j \rangle \to \psi_j$ and $\langle b_j^\dagger \rangle \to \psi_j^*$:

$$H_j^{MF}\left(\{\Psi_i\},\{\Psi_i^*\}\right) = -J\Big[\, b_j^\dagger \Big(\sum_{\substack{i\,NN\\ \text{of } j}} \Psi_i\Big) + \Big(\sum_{\substack{i\,NN\\ \text{of } j}} \Psi_i^*\Big) b_j \Big]$$

$$+ \frac{U}{2} n_j (n_j - 1)$$

(ii) Assume <u>homogeneous</u> order parameter $\Psi_i \to \Psi$,

i.e. $\displaystyle\sum_{\substack{i\,NN\\ \text{of } j}} \Psi_i = z\Psi$

#NN

$$\rightsquigarrow \quad H_j^{MF}(\Psi, \Psi^*) = -zJ\left[b_j^\dagger \Psi + \Psi^* b_j\right] + \frac{U}{2} n_j (n_j - 1)$$

dropped from now

(iii) Represent $H_j^{MF} - \mu n_j$ in occupation basis $\{|n\rangle^{(j)}\}$

$$\langle n | H_j^{MF} - \mu \hat{n}_j | m \rangle = \left(\frac{U}{2} n(n-1) - \mu n \right) \delta_{n,m}$$

$$- zJ \left[\psi \underbrace{\langle n | b_j^\dagger | m \rangle}_{= \sqrt{m+1}\, \delta_{n,m+1}} + \psi^* \underbrace{\langle n | b_j | m \rangle}_{= \sqrt{m}\, \delta_{n,m-1}} \right]$$

$\rightsquigarrow$ Matrix form:

$$\begin{array}{cc} \begin{pmatrix} 0 & -zJ\psi^* & & & \\ -zJ\psi & -\mu & -zJ\sqrt{2}\psi^* & & \\ & -zJ\sqrt{2}\psi & U-2\mu & -zJ\sqrt{3}\psi^* & \\ & & -zJ\sqrt{3}\psi & 3U-3\mu & \ddots \\ & & & \ddots & \ddots \end{pmatrix} & \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ \vdots \\ n_{max} \end{array} \end{array}$$

3. (i) Pick random initial Ψ

(ii) Solve $$\left(H_j^{MF} - \mu n_j\right)\begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_{n_{max}} \end{pmatrix} = \varepsilon \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_{n_{max}} \end{pmatrix}$$

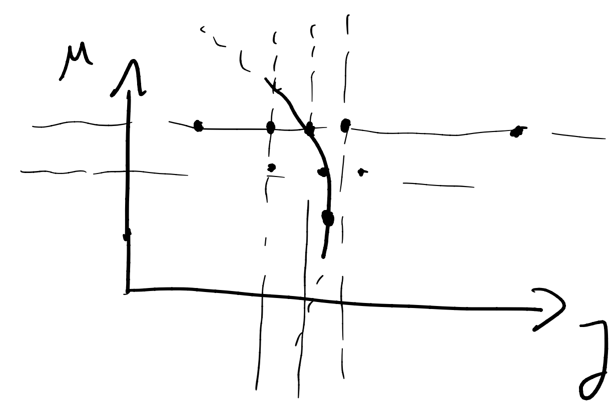
for groundstate with eigenvalue ε_0, and eigenstate $\begin{pmatrix} f_0^{(0)} \\ f_1^{(0)} \\ \vdots \\ f_{n_{max}}^{(0)} \end{pmatrix}$.

(iii) Update Ψ, Ψ^* in H_j^{MF} as $\Psi \rightarrow \sum_{n=0}^{n_{max}-1} f_n^{(0)*} f_{n+1}^{(0)} \widehat{T}_{n+1}$.

$$\Psi^* \rightarrow \sum_{n=1}^{n_{max}} f_n^{(0)*} f_{n-1}^{(0)} \widehat{T}_n$$

(iv) Return to (ii) and iterate until change in $|\Psi|$ is below a threshold $\delta \sim 10^{-10}$.

$\rightsquigarrow$ Map out self-consistent Ψ as a function of J/U and μ/U for fixed $U > 0$, either by discrete sampling of the parameter plane (J, μ), or by finding the transition line using nested intervals search:



4. Which n_{max} is sufficient?

Compare phase diagram for different values of n_{max} $\rightsquigarrow$ changes only occur when n_{max} comes close to

$\frac{\mu_{max}}{U}$. See attached plots for illustration.

Data on z=2 (1D)

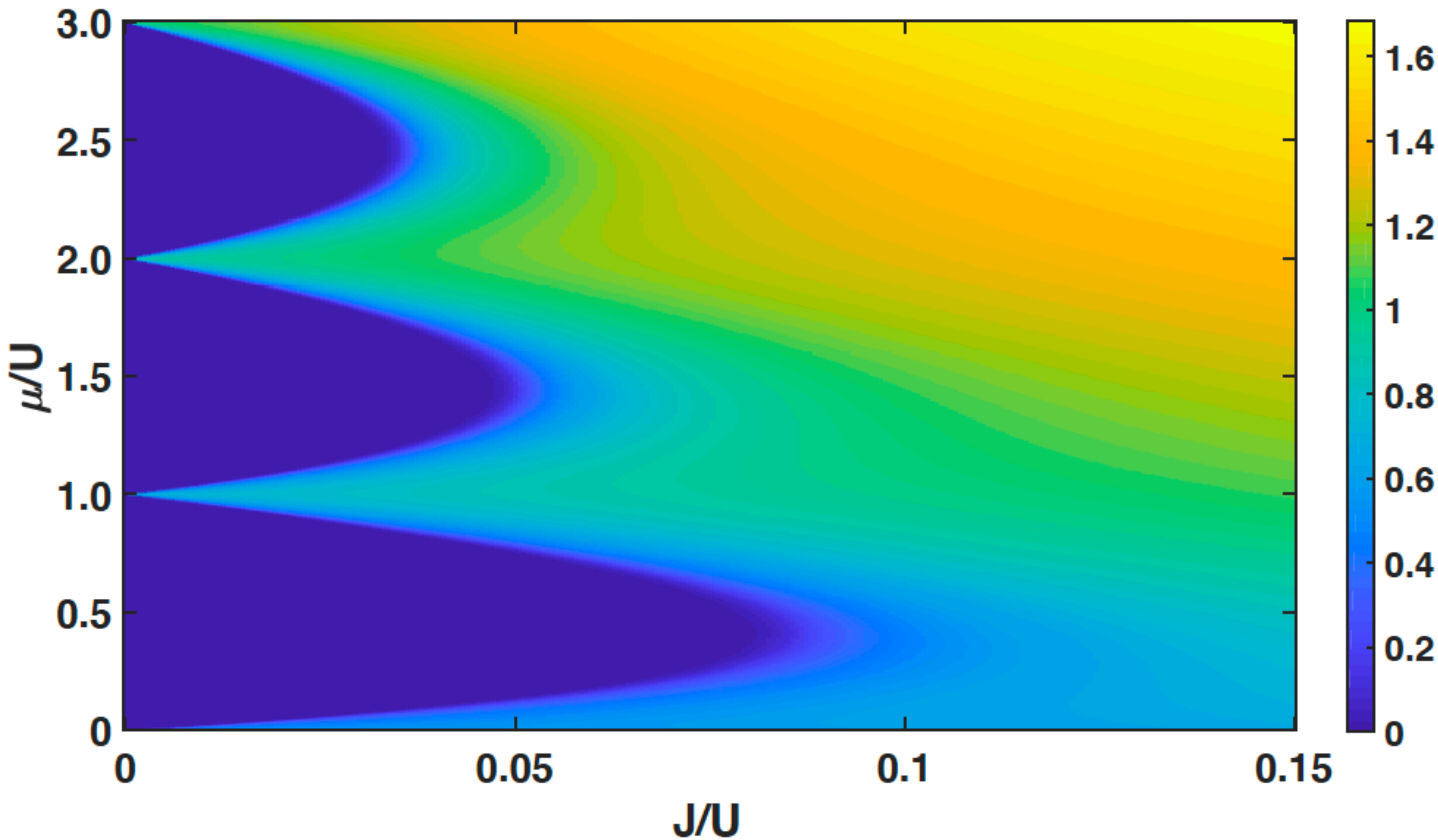
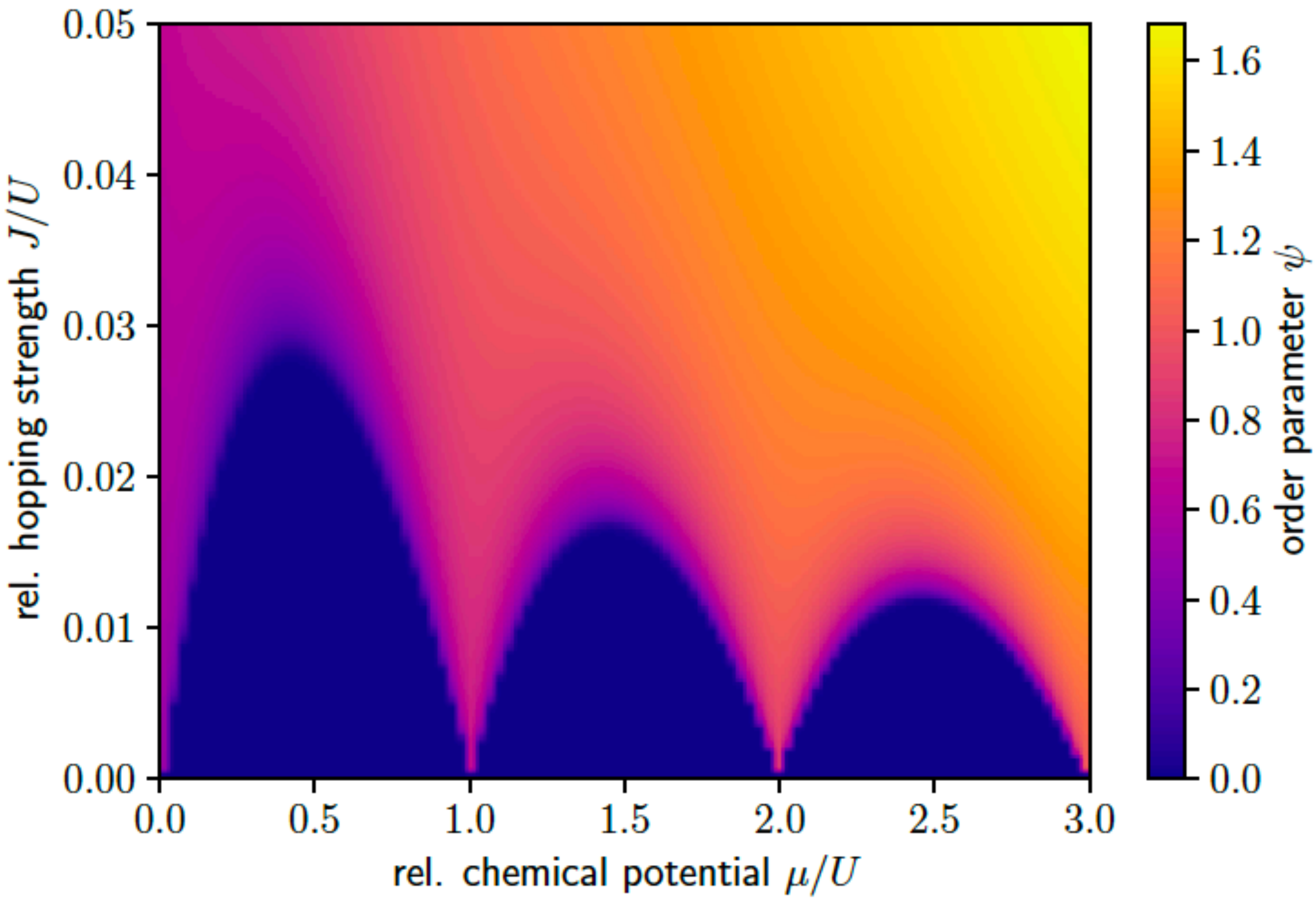


Figure 1: Phase diagram of the one-dimensional Bose-Hubbard model in the mean-field approximation. The blue "Mott lobes" where $\psi \sim 0$ correspond to the Mott insulating phase. For sufficiently strong hopping J, a transition to a superfluid phase happens, where $\psi \neq 0$. Here $n_{max} = 8$.

Data on z=6 (3D cubic)



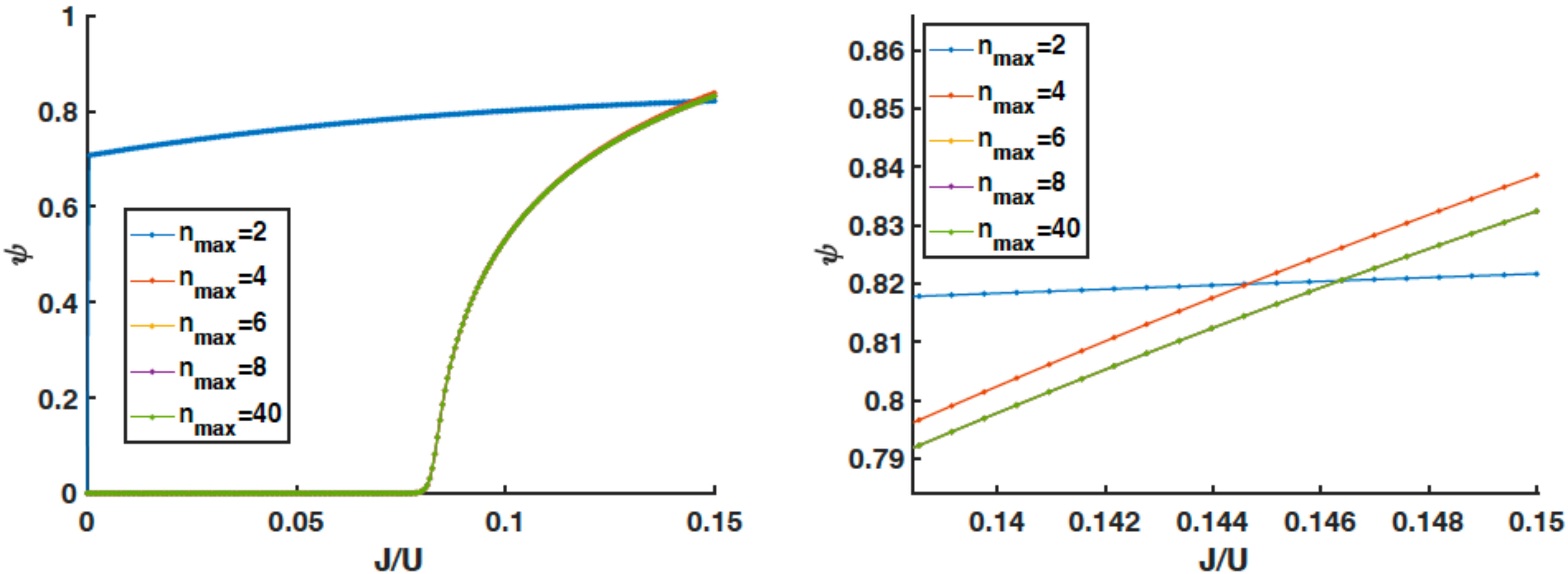
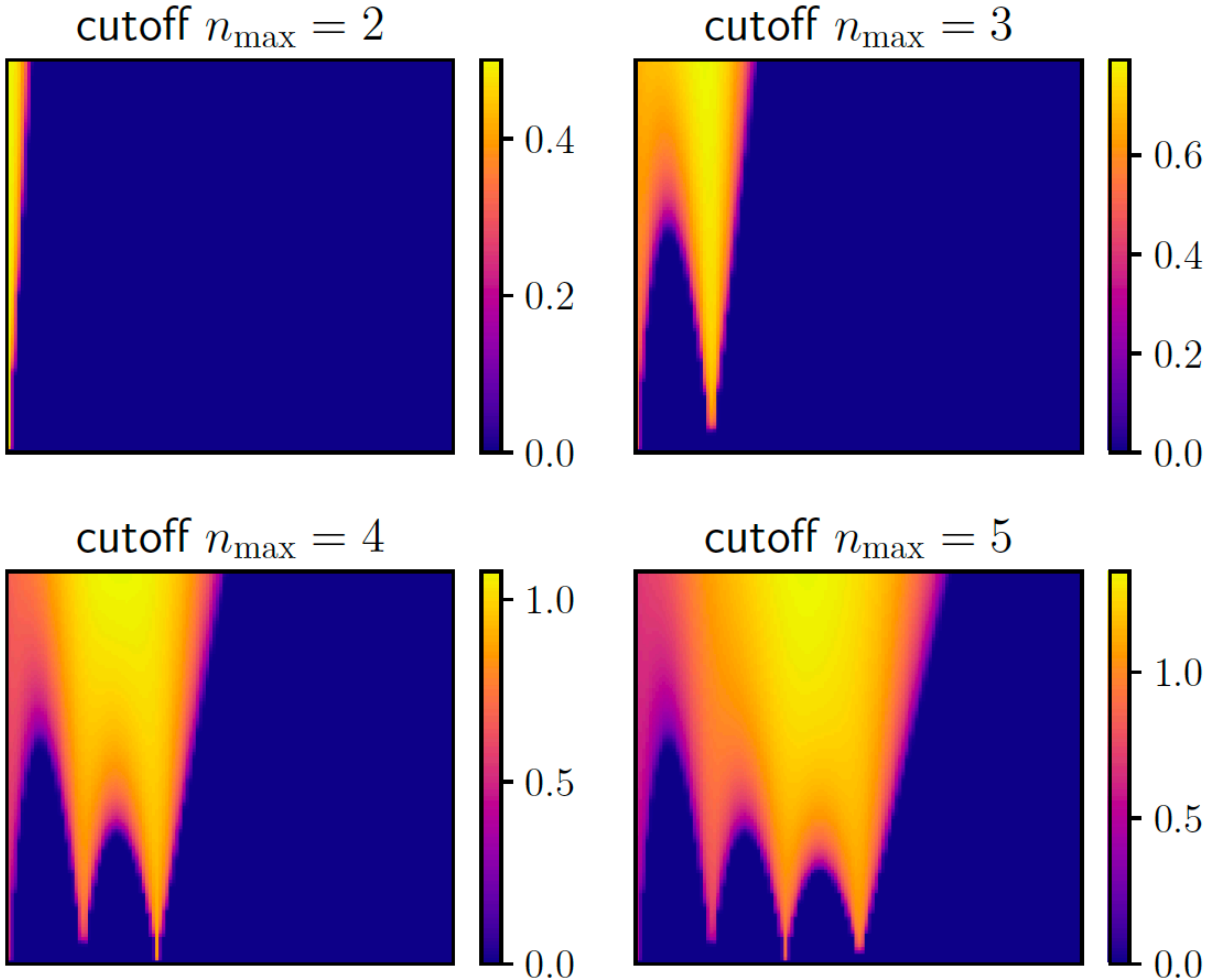
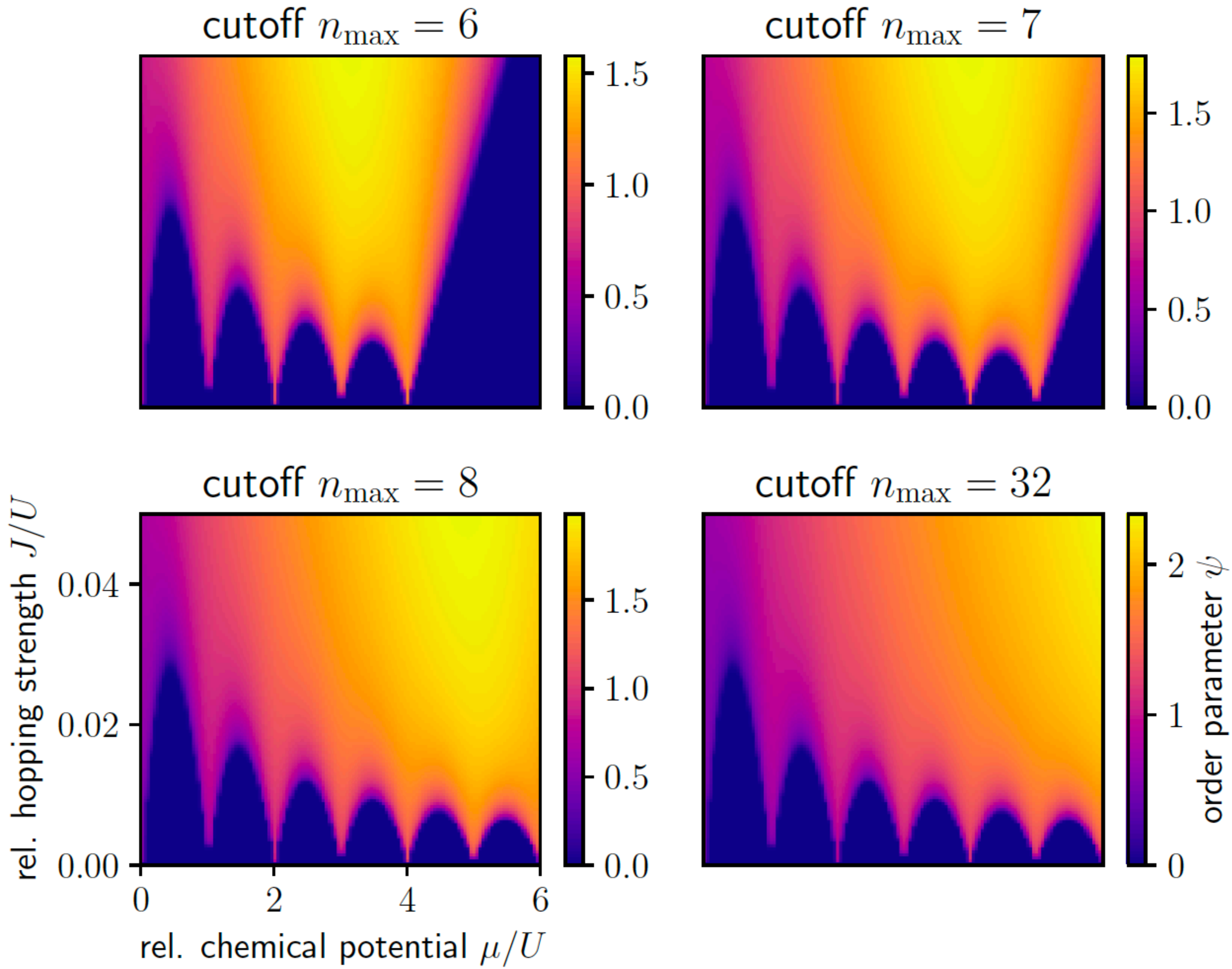


Figure 2: Convergence check with respect to the truncation n_{max} in the number of bosons per site. Here, ψ is computed for fixed $\mu/U = 0.5$ and $J/U \in [0, 0.15]$ (a horizontal line in the phase diagram above). For $n_{max} \geq 6$, changes to the results become insignificant.



cutoff $n_{\max} = 2$
0.0
0.2
0.4
cutoff $n_{\max} = 3$
0.0
0.2
0.4
0.6
cutoff $n_{\max} = 4$
0.0
0.5
1.0
cutoff $n_{\max} = 5$
0.0
0.5
1.0


cutoff $n_{\max} = 6$
cutoff $n_{\max} = 7$
cutoff $n_{\max} = 8$
cutoff $n_{\max} = 32$
rel. hopping strength J/U
rel. chemical potential μ/U
order parameter ψ
0.00
0.02
0.04
0
2
4
6
0.0
0.5
1.0
1.5
0
1
2