1. The multinomial ansatz

We derive this ansatz by looking at the non-interacting Bose Hubbard model with N particles in M modes. In momentum space, its ground state is

$$|\Phi\rangle = \frac{1}{\sqrt{N!}}\left(\hat{c}_0^\dagger\right)^N |\text{vac}\rangle\,, \tag{1}$$

where $\hat{c}_i^\dagger$ is the momentum space creation operator. Applying the Fourier transform to the above equation yields

$$|\Phi\rangle = \frac{1}{\sqrt{N!}}\left[\frac{1}{\sqrt{M}}\sum_{i=1}^{M}\hat{a}_i^\dagger\right]^N |\text{vac}\rangle\,, \tag{2}$$

where $\hat{a}_i^\dagger$ is the real space creation operator. Using the multinomial theorem, this can be rewritten as

$$|\Phi\rangle = \frac{N!}{\sqrt{N!M^N}} \sum_{(\nu_i\in\mathbb{N}_0)_{i=1}^M, \sum_{i=1}^M \nu_i = N} \prod_{i=1}^{M} \frac{1}{\nu_i!}\left(\hat{a}_i^\dagger\right)^{\nu_i}|\text{vac}\rangle \tag{3}$$

where the sum goes over all M-tuples of non-negative integers $(\nu_1, \nu_2, \ldots, \nu_M)$, whose elements sum to N. We rewrite (3) in terms of Fock states

$$|f\rangle = |\nu_1, \nu_2, \ldots, \nu_M\rangle = \prod_{i=1}^{M}\frac{1}{\sqrt{\nu_i!}}\left(\hat{a}_i^\dagger\right)|\text{vac}\rangle\,, \tag{4}$$

yielding the final form of the ansatz

$$|\Phi\rangle = \sqrt{\frac{N!}{M^N}}\sum_{|f\rangle}\left(\prod_{i=1}^{M}\frac{1}{\sqrt{\nu_i!}}\right)|f\rangle\,. \tag{5}$$

For use with importance-sampled FCIQMC, it is useful to introduce a parameter p to Eq. (5):

$$|\Phi(p)\rangle = \mathcal{N}\sum_{|f\rangle}\left(\prod_{i=1}^{M}\frac{1}{\nu_i!}\right)^p|f\rangle\,, \tag{6}$$

where $\mathcal{N}$ is an unknown normalization constant. How the parameter affects the result is shown in Fig. 1.

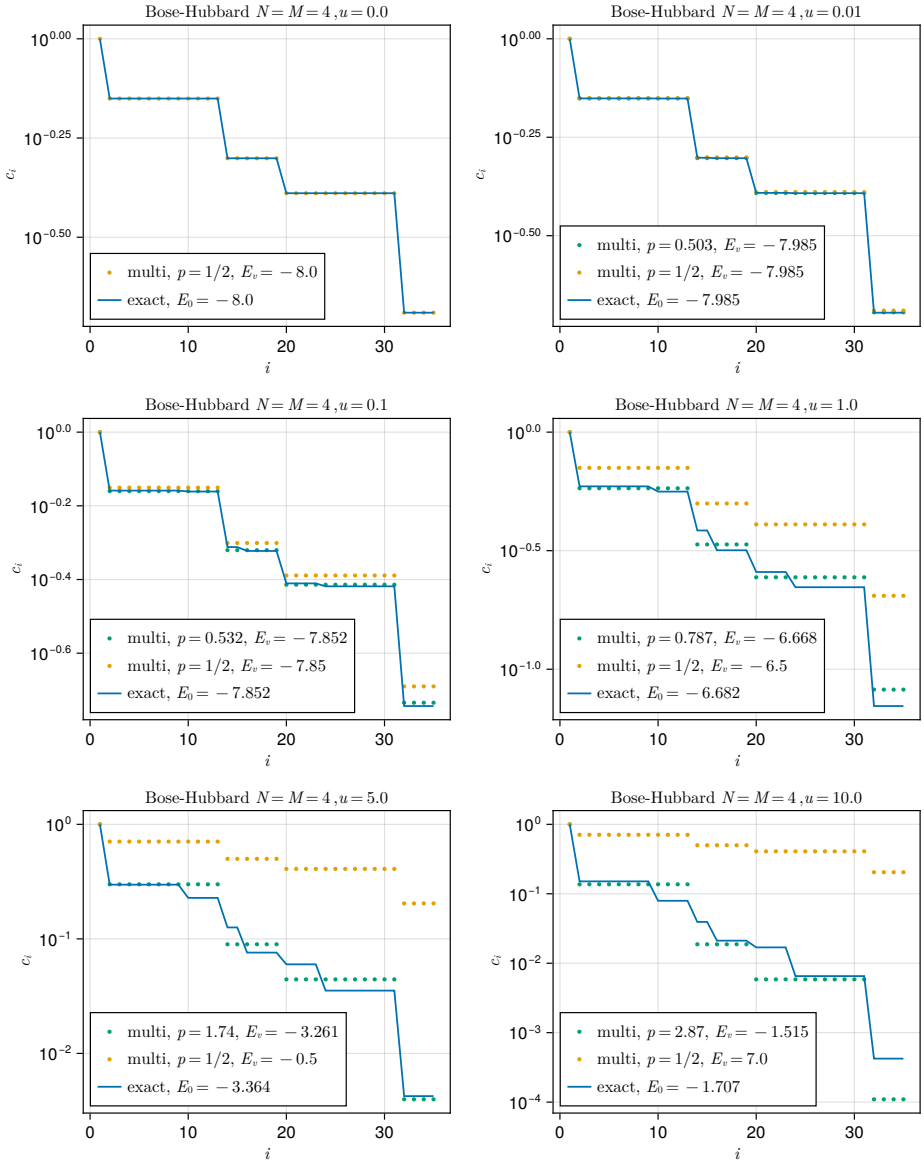

FIGURE 1. Comparison of the multinomial ansatz to the exact ground states of 1D Bose-Hubbard Hamiltonians with $N = 4$ particles in $M = 4$ sites and various interaction strengths u. The plot displays the coefficients of the true ground state eigenvector (labelled as exact), and the multinomial ansatz (Eq. (6)) with an optimal value of p, and with $p = 1/2$ (as seen in Eq. (5)). The vector indices i are ordered by the value of the ground state eigenvector.