Simulation of boson dynamics: A coherent-states-based method

Michal Horanský

University of Leeds

January 31, 2025

Introduction

Curse of dimensionality

- A system governed by a Hamiltonian \hat{H} which preserves the total particle number S across all M modes.
- We wish to find the time evolution of some quantum state $|\Psi\rangle.$
- ► The Hilbert space is spanned by an occupancy number basis of dimension

$$\dim(\mathcal{H}) = {S+M-1 \choose M-1}$$

which grows exponentially with M.

Introduction

Coherent states: construction

- Since H preserves S, its second quantization depends only on the dynamical operators $\hat{a}_i^{\dagger}\hat{a}_j$, which form the Lie algebra for the dynamical group $G = SU(M) \otimes U(1)$.
- ▶ \mathcal{H} is spanned by the elements of G acting on some reference state $|\Psi_0\rangle$, here chosen to be $|0,\dots 0,S\rangle$ —hence \hat{g} $|\Psi_0\rangle$ forms a basis to \mathcal{H} .
- ► There exists a stability subgroup $S \subset G$ which leaves $|\Psi_0\rangle$ invariant up to a constant factor.
- ▶ Hence a suitable (over-)complete basis is given by the unnormalized states $|z| = \exp\left[iz^i\hat{q}_i\right]|\Psi_0\rangle$, where \hat{q}_i is an element of the Lie algebra of the quotient group G/S.
- ▶ This is one way of constructing SU(M) coherent states.

Introduction

Coherent states: utility

- Coherent states evolve in a way that captures the dynamics of the Hamiltonian.
- For this reason, a small sample of coherent states should form a suitable basis for the propagation of $|\Psi\rangle$ (especially if the initial value of $|\Psi\rangle$ is highly localized in $|z\rangle$).
- ▶ Due to their structure, matrix elements of second-quantized Hamiltonians are easy to calculate in a coherent state basis.
- ▶ I chose to construct the states unnormalized, so that |z| has no explicit dependence on $\frac{\partial}{\partial z_i^*}$, allowing the use of Wirtinger calculus for the equations of motion.
- Even if the basis states are unnormalized, $|\Psi(t)\rangle$ remains normalized if we set the initial decomposition coefficients so that $\langle \Psi(t=0)|\Psi(t=0)\rangle=1$

Two applications

- I tried to reproduce two papers studying SU(M) Hamiltonians:
 - Qiao and Grossmann's paper on the Bose-Hubbard model
 - Green and Shalashilin's paper on bosons in a displaced harmonic trap
- ▶ For each of these Hamiltonians, I have simulated the time-evolution of an initially pure coherent state $|z_0|$ in two ways:
 - 1. Uncoupled basis: Each basis state is propagated separately $(\dim = M 1)$, then the decomposition coefficients are propagated on top of the evolved basis $(\dim = N)$.
 - 2. Variational method: The basis states and decomposition coefficients are fully coupled and propagated simultaneously $(\dim = N \cdot M)$.

Bose-Hubbard model - uncoupled basis propagation

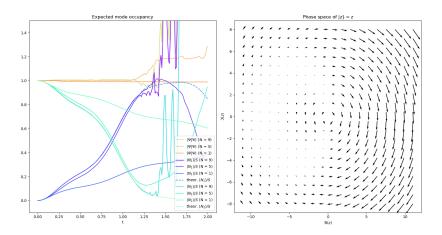


Figure: M = 2, S = 10, $|\Psi(t = 0)\rangle = n |0.0 + 0.0i\rangle$. $J(t) = 1 + \frac{1}{2}\cos(2\pi t)$, U = 0.1, K = 0

Bose-Hubbard model - fully variational method

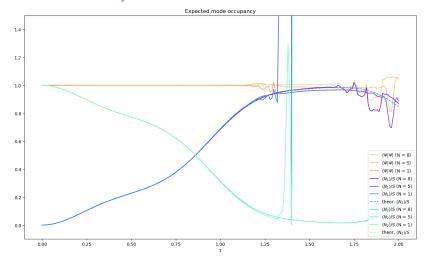


Figure:
$$M = 2$$
, $S = 10$, $|\Psi(t = 0)\rangle = n |0.0 + 0.0i\}$. $J(t) = 1 + \frac{1}{2}\cos(2\pi t)$, $U = 0.1$, $K = 0$

Bose-Hubbard model - uncoupled basis propagation

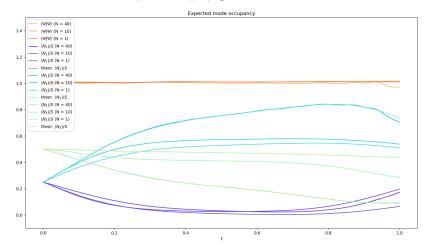


Figure:
$$M = 3$$
, $S = 10$, $|\Psi(t = 0)\rangle = n |0.0 + 0.0i\rangle$. $J(t) = 1 + \frac{1}{2}\cos(2\pi t)$, $U = 0.1$, $K = 0$

Bose-Hubbard model - fully variational method

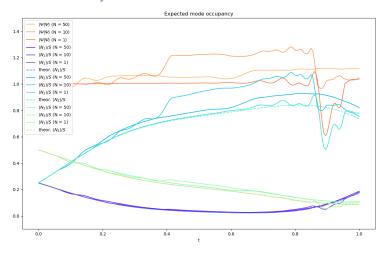


Figure:
$$M = 3$$
, $S = 10$, $|\Psi(t = 0)\rangle = n |0.5 + 0.5i, 0.5 - 0.5i\}$. $J(t) = 1 + \frac{1}{2}\cos(2\pi t)$, $U = 0.1$, $K = 0$

Displaced harmonic trap - uncoupled basis propagation

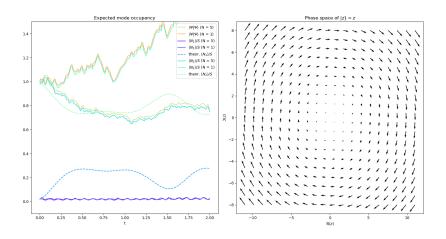
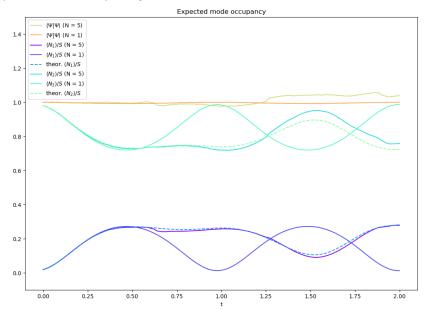


Figure: $M = 2, S = 10, |\Psi(t = 0)\rangle = n |0.1 + 0.1i\}$. $\xi = 2.1, \lambda_0 = 0.01$

Displaced harmonic trap - fully variational method



Displaced harmonic trap - fully variational method

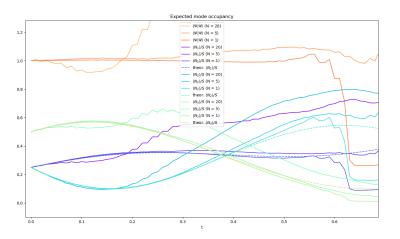


Figure:
$$M = 3$$
, $S = 10$, $|\Psi(t = 0)\rangle = n |0.5 + 0.5i, 0.5 - 0.5i\rangle$. $\xi = 2.1$, $\lambda_0 = 0.01$

Outlook

- Much faster (DHT with M=3: 1.5 minutes for an N=20 basis vs. 25 minutes for the occupancy basis solution)
- Numerically unstable (big M, big S, conditioning, regularisation...)
- Systems with different dynamical groups?

Thank you for your attention