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

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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
$$\dim(\mathcal{H}) = \binom{S+M-1}{M-1}$$
which grows exponentially with M.

- 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 $|0,\ldots 0, S\rangle$–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 $|z\}$).
- 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 $\langle\Psi(t=0)|\Psi(t=0)\rangle = 1$

Results so far

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 ($\dim = N \cdot M$).

Results so far

Bose-Hubbard model

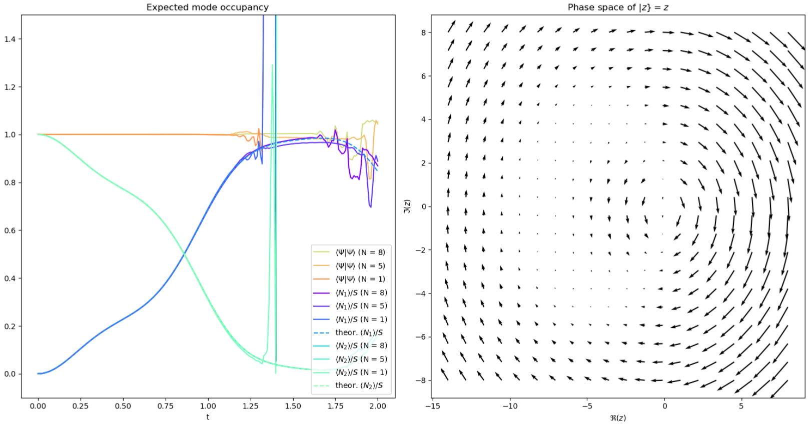

Figure: $M = 2, S = 10, |\Psi(t=0)\rangle = n\,|0.0 + 0.0i\}$.
$J(t) = 1 + \frac{1}{2}\cos(2\pi t), U = 0.1, K = 0$

Results so far

Bose-Hubbard model

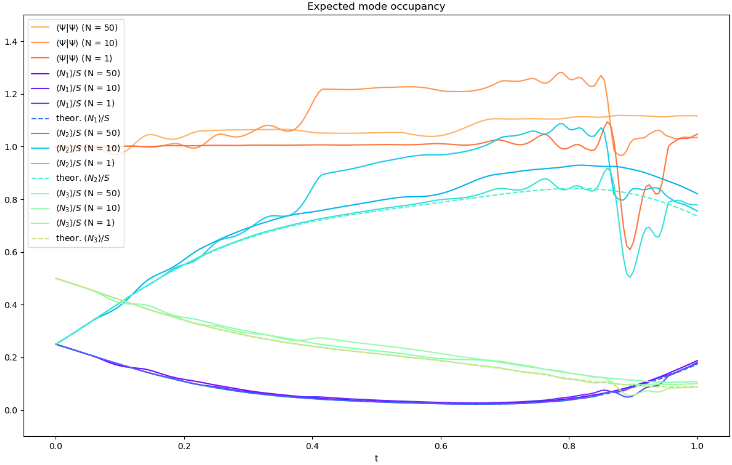

Figure: $M = 3, S = 10, |\Psi(t = 0)\rangle = n\,|0.5 + 0.5i, 0.5 - 0.5i\}$.
$J(t) = 1 + \frac{1}{2}\cos(2\pi t), U = 0.1, K = 0$

Results so far

Displaced harmonic trap

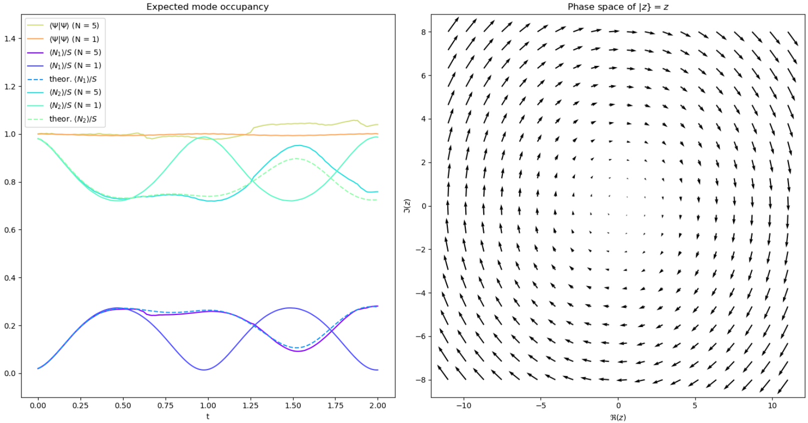

Figure: $M = 2, S = 10, |\Psi(t=0)\rangle = n\,|0.1 + 0.1i\}$. $\xi = 2.1, \lambda_0 = 0.01$

Results so far

Displaced harmonic trap

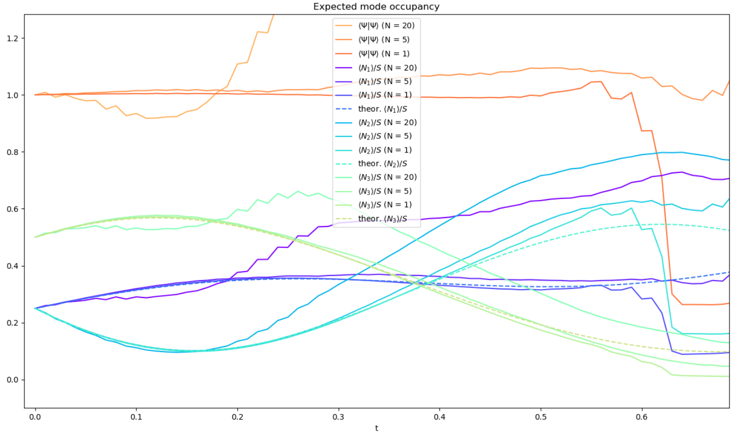

Figure: $M = 3, S = 10, |\Psi(t = 0)\rangle = n\,|0.5 + 0.5i, 0.5 - 0.5i\}$.
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Outlook

- 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