Bosonic and fermionic coherent states

A progress report

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June 20, 2025

Bosonic $SU(M)$ CSs

Progress on simulation of dynamics

- Numerical issues solved; the data for $M = 2, 3$ is now sensible
- Comparison with fully variational approach shows that the decoupled basis method reproduces the dynamics of a low-mode system sufficiently well–and saves a lot of time
- So far, the initial wavefunction was a "pure" coherent state, which will be pefectly reproduced by a basis of size 1 in the coherent timespan
- What to do next:
  - For arbitrary intitial wavefunctions, a sane sampling method must be implemented
  - Stability must be shown for large $(20 - 30)$ number of modes
  - Minimal required basis size for these cases is to be found

Fermionic $SU(M)$ CSs

Construction

- I found a construction of fermionic coherent states which
  1. is wholly contained in the particle-preserving Hilbert space
  2. doesn't use Grassmann algebra
- In this construction:
  - Each CS is parametrised by $S(M-S)$ complex parameters
  - The overlap $\langle Z_a | Z_b \rangle$ is calculable as a determinant in $O(M^3)$
  - The Hamiltonian matrix element $\langle Z_a | \hat{H} | Z_b \rangle$ is calculable as an M^4-term sum of determinant-like reduced overlaps, yielding a time complexity of $O(M^7)$.

Fermionic $SU(M)$ CSs

Utility

- Can be used to calculate the dynamics of a molecular electronic Hamiltonian with complexity polynomial in M
- This can be used to find the molecular ground state
- Example methods:
  - Krylov-Lanczos method
  - Imaginary time propagation

Outlook

- I am currently implementing a python framework to perform krylov-lanczos calculations on arbitrary molecules using the fermionic CS construction
- Other things which would be useful:
  - Can the Hamiltonain matrix element be calculated with smaller time complexity if optimised well?
  - Can a simple expression for the inverse of the Kähler potential of the fermionic $SU(M)$ CSs be found? (This would be equivalent to lowering the time complexity on single-CS dynamics calculations)
  - Formalism comparison with Dima

Thank you for your attention