Bosonic and fermionic particle-preserving coherent states, their dynamics and applications

Transfer Report

Michal Horanský

July 17, 2025

Abstract

Coherent states-based methods have been previously developed and utilised for particle-preserving bosonic systems, such as the Bose-Hubbard model. This work is divided into two parts: Firstly, a new method is proposed for the bosonic systems, where the basis coherent states are propagated separately to create a frozen dynamical basis, which lowers the time-complexity significantly. Second, an analogous method is proposed for particle-preserving fermionic systems, and particularly the electronic structure of a molecule, for which the goal of this method is to find the ground state. For this, multiple methods are outlined, and relevant properties of the fermionic coherent states are obtained.

Contents

Chapter 1

Background

To find the dynamics of a given system, one typically needs to solve the Schrodinger equation given by the system's Hamiltonian. For complex systems which can be found in nature, an analytic solution rarely exists. To solve this partial differential equation computationally, one needs to chose a basis for the Hilbert space and, since it typically is infinite or even continuous, sample it to obtain a basis sample onto which the initial state is decomposed and on which it is propagated. This sampling choice is always limiting and must be carefully justified, as omitting elements of the Hilbert space may render the analysis inaccurate.

Coherent states are particular states in the Hilbert space which follow classical trajectories, remain coherent, and minimise position-momentum uncertainty. Choosing them as the basis, a very small sample is typically suitable to capture the physics of a wide variety of systems and starting conditions [10]. This is an example of a semi-classical approximation.

1.1 Utility and scope of semi-classical methods

get that adiabatic shit outta here lil bro

1.1.1 Bosonic system 1: Bose-Hubbard model

he bossin

1.1.2 Bosonic system 2: Displaced harmonic trap

me when i quantise the modes

1.1.3 Fermionic system: molecular electronic structure

ground state would be nice aha

1.2 Coherent states: a hundred year-long history

The study of classical trajectories present in quantum dynamics dates back to Schrodinger's work in 1926, and remained an active area of study ever since. Multiple generalisations were constructed for the initial concept of coherent states, and the specific properties of coherent states of many particular systems were found and subsequently utilised in semi-classical methods. In this section, I outline a brief history of the theoretical treatment of coherent states leading up to the framework used for the $SU(M)$ bosonic/fermionic coherent states.

1.2.1 Schrodinger: the harmonic oscillator

In 1926, Schrodinger formulated so-called "classical states" of the simple harmonic oscillator [2]. Consider the Hamiltonian of the simple harmonic oscillator

$$\hat{H} = \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \tag{1.1}$$

where ω is the characteristic scale of the potential. Then consider the following superposition of energy eigenstates $|n\rangle$, characterised by a single complex parameter α:

$$|\alpha\rangle = N(\alpha) \sum_{i=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{1.2}$$

where $N(\alpha)$ is a normalisation factor. This state has the following properties:

1. The expected values of $\hat{x}$ and $\hat{p}$ are proportional to the real and imaginary components of α, respectively.
2. These expected values evolve according to the "classical" Hamiltonian equation, which can therefore be succintly written as

   $$\dot{\alpha} = -i \frac{\partial H(\alpha, \alpha^*)}{\partial \alpha^*} \tag{1.3}$$

   where $H(\alpha, \alpha^*)$ is the classical simple harmonic oscillator Hamiltonian as given by the expected values of $\hat{x}, \hat{p}$.
3. The position and momentum uncertainties of $|\alpha\rangle$ are minimal: $\Delta x \Delta p = \frac{1}{2}$.
4. The state remains "coherent", i.e. as it evolves, the parameter $\alpha(t)$ changes, but the wave-state remains describable by the construction in Eq. 1.2.

The significance of these states is immediately obvious: although fundamentally non-classical, the Schrodinger equation with the simple harmonic oscillator Hamiltonian permits "wave-groups" (as dubbed by Schrodinger) whose expectation values not only follow non-trivial classical trajectories, but which remain compact (both in space and in momentum representation!) and coherent.

1.2.2 Glauber: field coherent states

In 1963, Glauber generalised Schrodinger's construction to the Hamiltonian which describes the interaction between an atomic system and an electromagnetic field, forming field coherent states[1] [3]. According to Glauber, the following three properties all lead to the construction of field coherent states [7, p. 869]:

1. The coherent state is an eigenstate of the annihilation operator

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \tag{1.4}$$

2. The coherent state is obtained by applying a displacement operator on the vacuum state

$$|\alpha\rangle = \hat{D}(\alpha)\,|0\rangle \quad \text{where} \quad \hat{D}(\alpha) = \exp\bigl(\alpha\hat{a}^\dagger - \alpha^*\hat{a}\bigr) \tag{1.5}$$

3. The coherent state is a state with minimal position-momentum uncertainty.

However, as remarked by Zhang, Feng, and Gilmore in [7], the third property is not sufficient for a unique construction.

Field coherent states showed that "classical states" are present in systems beyond the simple harmonic oscillator, but Glauber's construction still was not applicable to general Hamiltonians–specifically, it fails when the Hilbert space is finite, as no eigenstate of the annihilation operator exists! This is particularly relevant when studying systems which preserve total particle number, and thus further generalisation was required.

1.2.3 Perelomov and Gilmore: generalised field coherent states

Such a generalisation of Glauber's coherent states for arbitrary Hamiltonians was indeed found independently by Perelomov [5] and Gilmore [6] in 1972. This construction discards the approach via annihilation operator eigenstates, and instead fully generalises the approach through the displacement operator (which, in retrospect, fully recovers Schrodinger's classical states and Glauber's field coherent states). Perelomov and Gilmore's construction follows these steps:

1. Firstly, the transition operators $\hat{T}_i$ of the Hilbert space $\mathcal{H}$ are identified. These are operators which, given any state in $\mathcal{H}$, can reach any other state in $\mathcal{H}$ by finitely-many sequential applications to the initial state. These operators must form a Lie algebra. Also, the Hamiltonian has to be expressable as a function of the transition operators (not necessarily a linear function).

2. Secondly, a reference state $|\phi_0\rangle$ is chosen. This choice is arbitrary.

[1] Also called Glauber coherent states.

3. Thirdly, two Lie groups are identified: the dynamical group G, which is the Lie group associated with the Lie algebra formed by the transition operators $\hat{T}_i$, and its stability subgroup $\hat{H}$, which is the group of all elements in G which leave $|\phi_0\rangle$ invariant up to a phase. The quotient group G/H then contains elements $\hat{D(z_j)} = \exp\left(\sum_j z_j \hat{T}_j\right)$, where the sum over j contains those transition operators which are not in the stability group Lie algebra. Thus we obtain a map which assigns one coherent state to every element of the quotient group:

$$|z\rangle = N(z, z^*) \exp\left(\sum_j z_j \hat{T}_j\right) |\phi_0\rangle \tag{1.6}$$

where N is a normalisation function, which is necessary since $\hat{D}(z)$ is not in general unitary: the parameters z_j are complex and the transition operators are not required to be Hermitian.

These states posses many of the aforementioned properties, most importantly, classical-like trajectories, as will be discussed in Sec. 1.3.

1.3 Mathematical approach to CS-based methods

In this section, we firstly discuss the mathematical properties of generalised field coherent states and their ensembles, and then the particular construction of $SU(M)$ coherent states.

1.3.1 Topology of the CS parameter space

This subsection is a summary of relevant information as included by Viscondi, Grigolo, and de Aguiar in their review of generalised field coherent states [8].

When applying the quotient-space displacement operator on the reference state, the resulting states are no longer normalised. We will adopt the notation of Viscondi, Grigolo, and de Aguiar, and denote unnormalised elements of the Hilbert space as bras and kets with curly brackets. Then, the unnormalised coherent state is directly obtained as

$$|z\} = \hat{D}(z)\,|\phi_0\rangle \tag{1.7}$$

and a normalised coherent state is constructed by scaling by a normalisation factor:

$$|z\rangle = N(z^*, z)\,|z\} \quad \text{where} \quad N(z_a^*, z_b) = \{z_a|z_b\}^{-\frac{1}{2}} \tag{1.8}$$

The quotient space can be characterised by the following metric:

$$g(z_a^*, z_b) = \frac{\partial^2 \ln \{z_a^*|z_b\}}{\partial z_b \partial z_a^*} \tag{1.9}$$

Then, the coherent states remain coherent under time evolution, with the parameter z evolving according to a Hamiltonian equation on a curved manifold:

$$\dot{z}_i = -i\xi_{ij}^T(z^*, z)\frac{\partial H(z^*, z)}{\partial z_j^*} \tag{1.10}$$

where $H(z^*, z) = \langle z|\hat{H}|z\rangle$ is the effective Hamiltonian and $\xi(z^*, z)$ is the inverse of the quotient-space metric $g(z^*, z)$.

1.3.2 Fully variational equations of motion

Here we employ the paradigm discussed in previous sections which encompasses the heart of this kind of semi-classical approaximation: a limited sample of classical trajectories. We will approximate our Hilbert space by a discrete sample of N coherent states, each characterised by its parameters z_a, which evolve in time. Onto this basis sample, we decompose an arbitrary wavestate $|\Psi(t = 0)\rangle$ whose dynamics we are interested in:

$$|\Psi(t = 0)\rangle = \sum_{a=1}^{N} A_a(t = 0)\,|z_a(t = 0)\} \tag{1.11}$$

Note that I opt to use the unnormalised coherent states as the basis, rather than their normalised counterparts. This does not affect the physicality of the solution, which shall remain normalised, and it serves to simplify the equations of motion by omitting the normalisation factors $N(z_a)$.

Now, we can apply the Schrodinger Lagrangian $\hat{L} = i\frac{\mathrm{d}}{\mathrm{d}t} - \hat{H}$ onto our system of free coordinates (A_a, z_a) to obtain a system of first-order equations of motion, which can be computationally solved to obtain the trajectories of the basis, the decomposition coefficient evolution, and hence the evolution of the initial wavestate. This approach is a slight modification of the approach used by Qiao and Grossmann in [10].

Let us begin by obtaining the derivatives of unnormalised coherent states:

$$\frac{\partial}{\partial z_j} |z\} = \frac{\partial}{\partial z_j} \exp\left(z_i \hat{T}_i\right) |\phi_0\rangle = \hat{T}_j |z\} \tag{1.12}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} |z\} = \frac{\mathrm{d}}{\mathrm{d}t} \exp\left(z_i \hat{T}_i\right) |\phi_0\rangle = \dot{z}_i \hat{T}_i |z\} \tag{1.13}$$

1.3.3 $SU(M)$ coherent states

Chapter 2

Current work

i work hard yes

2.1 Bosonic $SU(M)$ coherent states

2.1.1 Construction

transitioning into a better person rn

2.1.2 Results

2.2 Fermionic $SU(M)$ coherent states

2.2.1 Construction of the unnormalised state

2.2.2 Overlap and normalisation

2.2.3 Fermionic operator sequence matrix element

2.2.4 Connection to molecular electronic structure

quote the two body and one body integrals matey

2.2.5 How to get that sweet sweet ground state

Chapter 3

Outlook

we want that nobel ngl

Bibliography

[1] Shalashilin, D. V. (2011), Multiconfigurational Ehrenfest approach to quantum coherent dynamics in large molecular systems. *Faraday Discussions*, **153**, pp. 105–116

[2] Schrodinger, E. (1926), Der stetige übergang von der Mikro-zur Makromechanik. *Naturwiss.* 14, pp. 664-666. Translated into English in Schrodinger, E. (1928), *Collected Papers in Wave Mechanics*. 1st edn. London: Blackie & Son, pp. 41–44

[3] Glauber, R. J. (1963), Coherent and Incoherent States of the Radiation Field. *Phys. Rev.*, **131**, 6, pp. 2766–2788

[4] Klauder, J. R., Skagerstam, B. S. (1985), *Coherent States: Applications in Physics and Mathematical Physics*. 1st eng. edn. Singapore: World Scientific.

[5] Perelomov, A. M. (1972), Coherent states for arbitrary Lie group. *Commun. Math. Phys.*, **26**, pp. 222–236

[6] Gilmore, R. (1972), Geometry of symmetrized states. *Ann. Phys.*, **74**, 2, pp. 391–463

[7] Zhang, W. M., Feng, D. H., Gilmore, R. (1990), Coherent states: Theory and some applications. *Rev. Mod. Phys.*, **62**, pp. 867–927

[8] Viscondi, T. F., Grigolo, A., de Aguiar, M. A. M. (2015), Semiclassical Propagator in the Generalized Coherent-State Representation. arXiv:1510.05952 [**quant-ph**]

[9] Block, I., Dalibard, J., Zwerger, W. (2008), Many-body physics with ultracold gases. *Rev. Mod. Phys.*, **80**, pp. 885–964

[10] Qiao, Y., Grossmann, F. (2021), Exact variational dynamics of the multimode Bose-Hubbard model based on $SU(M)$ coherent states. *Phys. Rev. A*, **103**, 042209

[11] Green, J. A., Shalashilin, D. V. (2019), Simulation of the quantum dynamics of indistinguishable bosons with the method of coupled coherent states. *Phys. Rev. A*, **100**, 013607

[12] Bertlmann, R. A., Krammer, P. (2008), Bloch vectors for qudits. arXiv:0806.1174 **[quant-ph]**

[13] Buonsante, P., Penna, V.(2008), Some remarks on the coherent-state variational approach to nonlinear boson models. *J. Phys. A: Math. Theor.*, **41**, 175301

[14] Grigolo, A., Viscondi, T. F., de Aguiar, M. A. M. (2016), Multiconfigurational quantum propagation with trajectory-guided generalized coherent states. *J. Chem. Phys.*, **144**, 094106

Appendix A

Auxilary theorems

This appendix presents mathematical results which were used to derive the mathematical properties of bosonic and fermionic coherent states, but which were chosen to be omitted from the main body of text due to their abstract mathematical nature.

The author does not claim originality of these theorems or their proofs, but chooses to include them, as he was unable to find them in existing literature. The work presented in this appendix is the author's, except for mathematical identities which are stated explicitly.

A.1 counting minors