

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

Transfer Report

Michal Horanský

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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.

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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 choose 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 [13]. This is an example of a semi-classical approximation.

1.1 Utility and scope of semi-classical methods

Semi-classical methods have long been used in computational quantum dynamics, mainly in systems which can be partitioned into multiple sub-systems, some to be treated classically, some to be treated with the machinery of quantum mechanics [2]. A common example is the molecule, for which, based on the Born-Oppenheimer approximation, the nuclei may be treated as if following classical trajectories, and the electronic structure following quantum dynamics.

More recently, systems which are "fully quantum" started being approached with classical approach in mind, as quantum dynamics may be formulated on top of classical behaviour embedded in a quantum-mechanical system [3].

An example of this approach is the method of coherent-state basis trajectories, which lies at the heart of my research. As elaborated on below in Sec. 1.2, states which follow classical-like trajectories and which remain localised in phase-space are embedded in every quantum system, and are inextricably linked to second-quantisation of position and momentum operators. This second-quantisation expresses the state of a system by the level of discrete excitations in an array of modes. As such, we have chosen three particular physical systems as subjects to the methods developed in this work: two analysing bosonic dynamics, and one analysing fermionic dynamics.

1.1.1 Bosonic system 1: Bose-Hubbard model

The Bose-Hubbard model describes the physics of bosonic particles trapped on a lattice, which is for our particular analysis chosen to be one-dimensional. The modes occupied by a fixed total number of bosons correspond to sites on this lattice, and the relevant components of the Hamiltonian are on-site energy U and hopping energy J , respectively. The model, in its general formulation, also incorporates an external potential being applied on the lattice, which we, however, ignore. As such, the full Hamiltonian becomes:

$$\hat{H} = -J \sum_{i=1}^{M-1} \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_{i+1}^\dagger \hat{b}_i \right) + \frac{U}{2} \sum_{i=1}^M \hat{b}_i^\dagger{}^2 \hat{b}_i^2 \quad (1.1)$$

This system has previously been analysed using coherent-states-based methods by Qiao and Grossmann [13]. As such, the machinery we propose for bosonic systems shall be compared to this work as a benchmark.

The method used by Qiao and Grossmann is as follows: a basis of generalised field coherent states is constructed mathematically and then sampled around the initial wavestate. The elements of this basis are parametrised by complex vectors $\vec{\xi}_a$. The wavestate is decomposed into this basis like so:

$$|\Psi\rangle = \sum_a^N A_a \left| \vec{\xi}_a \right\rangle \quad (1.2)$$

where $A_a, \vec{\xi}_a$ are taken as dynamical coordinates. The equations of motion for these coordinates are expressed in a fully variational manner from the Schrodinger Lagrangian, and solved numerically as an initial-value problem for several particular choices of system parameters; importantly, for two-mode and three-mode lattices.

The method we propose as a faster alternative is as follows: after sampling the coherent state basis, each element of this basis is propagated along its classical-like trajectory. Then, the wavestate is decomposed onto the basis, and its decomposition coefficients are propagated on this basis, which is not constant in time, but follows pre-determined trajectories. As such, this is not a fully variational method, and the consideration for quantum effects is fully engrossed in the propagation of decomposition coefficients alone. We propose that for the type of initial wavestates as analysed by Qiao and Grossmann, which are either pure coherent states or superpositions of a handful of coherent states, this new method will converge easily with small basis samples and, by construction, entails drastically smaller time-complexity.

1.1.2 Bosonic system 2: Displaced harmonic trap

Another bosonic system is taken from the work of Green and Shalashilin [14], who studied a closed system of particles in a trap comprised of a displaced harmonic potential. This second application is of interest to us as a benchmark because it can be formulated with position and momentum operators, and the second-quantised formulation is in fact an alternative which requires a large number of modes (25–27) to converge. As such, the ability to solve this system with our new coherent-states-based method would prove its scalability for bosonic systems with a large number of modes.

The method utilised by Green and Shalashilin is similar to the one employed by us, but it is based on a less general formulation of coherent states, which are frozen gaussians in the phase space. As such, it serves as a useful benchmark in its own right to measure the trade-off between the accuracy of classical-like trajectories and added complexity of the more general formulation used in this work.

1.1.3 Fermionic system: molecular electronic structure

An example of a fermionic system which preserves the total number of particles is the electronic structure of an inert molecule. This is a very important problem, as the ground state of the electronic structure is closely related to many chemical properties of molecules. The molecular orbitals of electrons can be well-approximated as linear combinations of the electron orbitals of the constituent atoms [4].

In this work, we propose a new method for obtaining the ground state, which works by restricting the Hilbert space to a small coherent-state subspace surrounding the lowest-configuration state, sampling this subspace, and manually diagonalising the Hamiltonian

expressed as a matrix on the basis sample. One method for this is to take the lowest-configuration state as a reference state in our coherent state construction, which means it in itself is a coherent state, and then propagating it along its classical-like trajectory and sampling it at fixed time-intervals. Using the overcompleteness of coherent states, we hope that even a sample of a size much smaller than the dimensionality of the full Hilbert space will be able to converge to the true ground state.

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 [5]. Consider the Hamiltonian of the simple harmonic oscillator

$$\hat{H} = \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \quad (1.3)$$

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 :

$$|\alpha\rangle = N(\alpha) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (1.4)$$

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 succinctly written as

$$\dot{\alpha} = -i \frac{\partial H(\alpha, \alpha^*)}{\partial \alpha^*} \quad (1.5)$$

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. 1.4.

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 states¹ [6]. According to Glauber, the following three properties all lead to the construction of field coherent states [10, p. 869]:

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

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle \quad (1.6)$$

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

$$|\alpha\rangle = \hat{D}(\alpha) |0\rangle \quad \text{where} \quad \hat{D}(\alpha) = \exp(\alpha \hat{a}^\dagger - \alpha^* \hat{a}) \quad (1.7)$$

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

However, as remarked by Zhang, Feng, and Gilmore in [10], 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 [8] and Gilmore [9] 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.

¹Also 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 $D(\hat{z}_j) = \exp\left(\sum_j z_j \hat{T}_j\right)$, 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:

$$|z\rangle = N(z, z^*) \exp\left(\sum_j z_j \hat{T}_j\right) |\phi_0\rangle \quad (1.8)$$

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 possess 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 [11].

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

$$|z\rangle = \hat{D}(z) |\phi_0\rangle \quad (1.9)$$

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

$$|z\rangle = N(z^*, z) |z\rangle \quad \text{where} \quad N(z_a^*, z_b) = \{z_a | z_b\}^{-\frac{1}{2}} \quad (1.10)$$

The quotient space can be characterised by the following metric:

$$g(z_a^*, z_b) = \frac{\partial^2 \ln \{z_a^* | z_b\}}{\partial z_b \partial z_a^*} \quad (1.11)$$

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

$$\dot{z}_i = -i \xi_{ij}^T(z^*, z) \frac{\partial H(z^*, z)}{\partial z_j^*} \quad (1.12)$$

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 approximation: 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:

$$|\Psi(t=0)\rangle = \sum_{a=1}^N A_a(t=0) |z_a(t=0)\rangle \quad (1.13)$$

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 $\hat{L} = i\frac{d}{dt} - \hat{H}$ 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 [13].

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

$$\frac{\partial}{\partial z_j} |z\rangle = \frac{\partial}{\partial z_j} \exp(z_i \hat{T}_i) |\phi_0\rangle = \hat{T}_j |z\rangle \quad (1.14)$$

$$\frac{d}{dt} |z\rangle = \frac{d}{dt} \exp(z_i \hat{T}_i) |\phi_0\rangle = \dot{z}_i \hat{T}_i |z\rangle \quad (1.15)$$

Then the Lagrangian of the trial wavestate is

$$L = \sum_{m,n}^N \left(iA_m^* \dot{A}_n \{z_m|z_n\} + iA_m^* A_n \sum_i \dot{z}_{n,i} \{z_m|\hat{T}_i|z_n\} - \{z_m|\hat{H}|z_n\} \right)$$

and the equations of motion obtained by differentiating with respect to A_m^* , $z_{m,i}^*$, respectively, are

$$i \sum_n^N \left(\dot{A}_n \{z_m|z_n\} + A_n \sum_i \dot{z}_{n,i} \{z_m|\hat{T}_i|z_n\} \right) = \sum_n^N A_n \{z_m|\hat{H}|z_n\} \quad (1.16)$$

$$iA_m^* \sum_n^N \left(\dot{A}_n \{z_m|\hat{T}_i^\dagger|z_n\} + A_n \sum_j \dot{z}_{n,j} \{z_m|\hat{T}_i^\dagger \hat{T}_j|z_n\} \right) = A_m^* \sum_n^N A_n \{z_m|\hat{T}_i^\dagger \hat{H}|z_n\} \quad (1.17)$$

Note that for $N = 1$ (i.e. the wavestate is a pure coherent state), these equations are equivalent to Eq. 1.12.

It is helpful to express this in matrix form, with the coordinate vector defined as

$$\vec{Q} = \begin{pmatrix} \vec{Q}^A \\ \vec{Q}^z \end{pmatrix} \quad \vec{Q}_m^A = A_m \quad \vec{Q}^z = \begin{pmatrix} \vdots \\ \vec{Q}^{z,i} \\ \vdots \end{pmatrix} \quad \vec{Q}_m^{z,i} = z_{m,i} \quad (1.18)$$

where the first-order matrix equation of motion becomes

$$i\Omega \frac{d}{dt} \vec{Q} = \vec{R} \quad \text{where} \quad \vec{R} = \begin{pmatrix} \vec{R}^A \\ \vec{R}^z \end{pmatrix} \quad \vec{R}^z = \begin{pmatrix} \vdots \\ \vec{R}^{z,i} \\ \vdots \end{pmatrix} \quad (1.19)$$

and where

$$\Omega = \begin{pmatrix} \Omega^{AA} & \Omega^{A,1} & \dots & \Omega^{A,j} & \dots \\ \Omega^{1,A} & \Omega^{1,1} & \dots & \Omega^{1,j} & \dots \\ \vdots & \vdots & \ddots & \vdots & \\ \Omega^{i,A} & \Omega^{i,1} & \dots & \Omega^{ij} & \dots \\ \vdots & \vdots & & \vdots & \ddots \end{pmatrix} \quad (1.20)$$

The particular elements of the dynamical matrix Ω and the weight vector \vec{R} are then identified as

$$\Omega_{mn}^{AA} = \{z_m | z_n\} \quad (1.21)$$

$$\Omega_{mn}^{A,i} = A_n \{z_m | \hat{T}_i | z_n\} \quad \text{and} \quad \Omega^{i,A} = (\Omega^{A,i})^\dagger \quad (1.22)$$

$$\Omega_{mn}^{ij} = A_m^* A_n \{z_m | \hat{T}_i^\dagger \hat{T}_j | z_n\} \quad (1.23)$$

$$R_m^A = \sum_n^N A_n \{z_m | \hat{H} | z_n\} \quad (1.24)$$

$$R_m^{z,i} = A_m^* \sum_n^N A_n \{z_m | \hat{T}_i^\dagger \hat{H} | z_n\} \quad (1.25)$$

Note that A_m^* could have been factored out of the second group of equations, but was deliberately left in to demonstrate that Ω is Hermitian.

This form of the equation of motion is especially useful, since it yields itself readily to primitive methods of numerical integration (the method of choice in this work is the Dormand-Prince method, see below). To propagate the wavestate by a finite time-difference Δt , one simply inverts the dynamical matrix Ω at the current time. Therefore the time complexity of this approach is limited by the evaluation of R and Ω and the inversion of Ω , both of which are polynomial in the basis size and the number of transition operators.

1.3.3 $SU(M)$ coherent states

Consider a system characterised by M modes and S particles, with both of these numbers remaining constant. The most general transition operator is then

$$\hat{T}_{ij} = \hat{a}_i^\dagger \hat{a}_j \quad (1.26)$$

where we remain agnostic about whether \hat{a} denotes the bosonic or the fermionic annihilation operator. In either case, applying this operator on an arbitrary occupancy basis state within the configuration space yields either zero or another basis state within the configuration space. It can also be shown by applying the bosonic and fermionic commutation relations

that for both of these cases, the transition operators satisfy the following commutation relations:

$$[\hat{T}_{ij}, \hat{T}_{i'j'}] = \hat{T}_{ij'}\delta_{i'j} - \hat{T}_{i'j}\delta_{ij'} \quad (1.27)$$

Since the commutator is contained in the vector space spanned by \hat{T} , the transition operators form a Lie algebra.

On transformations of the dynamical Lie algebra

Note that a coherent state with parameter z is specified by the linear combination $z_i \hat{T}_i$. Hence, we can specify a new dynamical Lie algebra \hat{T}'_i formed as an arbitrary complex linear combination of \hat{T}_i . These two Lie algebras correspond to the same coherent state space, with the parametric maps related by the same linear transformation.

Firstly, we choose to transform the mode-number operators $\hat{a}_i^\dagger \hat{a}_i$ like so:

$$\hat{S} = \sum_i^M \hat{a}_i^\dagger \hat{a}_i \quad (1.28)$$

$$\hat{H}_i = \hat{a}_{i+1}^\dagger \hat{a}_{i+1} - \hat{a}_i^\dagger \hat{a}_i, \quad i = 1, 2 \dots M-1 \quad (1.29)$$

The operator \hat{S} is uninteresting, because every state in the configuration space is its eigenstate with eigenvalue S , and therefore \hat{S} is always in the stability subgroup. We can therefore ignore it.

The transformed Lie algebra constitutes the generators of real traceless $(M \times M)$ matrices, and therefore the full dynamical group is $U(1) \times SL(M, \mathbb{R})$. Ignoring the $U(1)$ direct product, as it is always fully contained in the stability subgroup, we may denote the dynamical group simply as $SL(M, \mathbb{R})$.

On the difference between $SU(M)$ and $SL(M, \mathbb{R})$

When transforming the basis \hat{T}_{ij} , one may choose to complexify it and form a set of Hermitian and anti-Hermitian operators $(\hat{T}_{ij} + \hat{T}_{ji}$ and $i(\hat{T}_{ij} - \hat{T}_{ji}))$, respectively. This complexification is allowed in the sense that the resulting coherent state space is equivalent. Identifying the resulting operators with the generalised Gell-Mann matrices yields the dynamical group $SU(M)$ [15]. Although resulting in a different quotient group G/H , the coherent states are identical to our $SL(M, \mathbb{R})$ construction. For the details of this construction, see Sec. 2.2.3 in the paper by Viscondi, Grigolo, and de Aguiar [11].

For the sake of simplicity and adherence to existing literature, we will refer to this construction as $SU(M)$ coherent states, but we will still use the exponential map with the $SL(M, \mathbb{R})$ generators, as it leads to much simpler mathematical treatment.

1.3.4 General approach to particle-preserving CS decomposition

This method is based on the approach in [16, App. E]. Suppose we have a reference state $|\phi_0\rangle$, and the quotient space of the dynamical group of some system is transversed by the exponential map of the operator $\hat{D}(z)$, so that

$$|z\rangle = e^{\hat{D}(z)} |\phi_0\rangle \quad (1.30)$$

and $\hat{D}(z)$ is a linear combination of transition operators which all destroy the vacuum state². Define $\hat{\phi}_0$ as such an operator so that

$$\hat{\phi}_0 |\text{vac.}\rangle = |\phi_0\rangle \quad (1.31)$$

Then we can write

$$|z\rangle = e^{\hat{D}(z)} \hat{\phi}_0 e^{-\hat{D}(z)} |\text{vac.}\rangle \quad (1.32)$$

using the fact that $\hat{D}(z) |\text{vac.}\rangle = 0$. We now express the operator product using Hadamard's lemma:

$$e^{\hat{D}(z)} \hat{\phi}_0 e^{-\hat{D}(z)} = \sum_{r=0}^{\infty} \frac{1}{r!} \left[\hat{D}(z), \hat{\phi}_0 \right]_r \quad (1.33)$$

where

$$\left[\hat{A}, \hat{B} \right]_r = \left[\hat{A}, \left[\hat{A}, \hat{B} \right]_{r-1} \right] \quad \text{and} \quad \left[\hat{A}, \hat{B} \right]_0 = \hat{B} \quad (1.34)$$

are the repeated commutators. The unnormalised coherent state is obtained by acting with this sum on the vacuum state.

²This is characteristic of dynamical groups which preserve total particle number.

Chapter 2

Current work

In this chapter I outline the application of the mathematical construction of $SU(M)$ coherent states in particular to bosonic systems (such as the ones described in Sec. 1.1.1, 1.1.2) and fermionic systems (such as the one described in Sec. 1.1.3).

2.1 Bosonic $SU(M)$ coherent states

2.1.1 Construction

In this subsection, I describe the properties of $SU(M)$ coherent states constructed on bosonic annihilation and creation operators.

Reference state and displacement operator

A suitable reference state for a bosonic system of M modes and S particles is

$$|\phi_0\rangle = |0, 0 \dots 0, S\rangle \quad (2.1)$$

Finding the stability subgroup of the dynamical group for this reference state, we ultimately obtain the displacement operator

$$\hat{D}(z) = \exp\left(\sum_{i=1}^{M-1} z_i \hat{b}_i^\dagger \hat{b}_M\right) \quad (2.2)$$

The bosonic $SU(M)$ coherent state is then

$$|z\rangle = N(z) \exp\left(\sum_{i=1}^{M-1} z_i \hat{b}_i^\dagger \hat{b}_M\right) |\phi_0\rangle \quad (2.3)$$

where z is a vector of $M - 1$ complex parameters

Decomposition into the occupancy basis

As shown by Buonsante and Penna in [16], this coherent state can be decomposed into the occupancy basis as follows:

$$|\vec{z}\rangle = \frac{N(z)}{\sqrt{S!}} \left(\hat{a}_M^\dagger + \sum_i^{M-1} z_i \hat{a}_i^\dagger \right)^S |0, 0 \dots 0\rangle \quad (2.4)$$

This result can be obtained by following the method outlined in Sec. 1.3.4. Applying the multinomial theorem gives the explicit superposition of occupancy basis states equivalent to the coherent state:

$$|z\rangle = N(z) \sum_{k_1+k_2+\dots+k_M=S} \sqrt{\frac{S!}{k_1!k_2!\dots k_M!}} z_1^{k_1} z_2^{k_2} \dots z_{M-1}^{k_{M-1}} |k_1, k_2 \dots k_M\rangle \quad (2.5)$$

Overlap and normalisation

Using Eq. 2.4 and Wick's theorem, the overlap of two bosonic CSs can be shown [13] to be

$$\langle z_a | z_b \rangle = N(z_a)N(z_b) \left(1 + \sum_i^{M-1} z_{a,i}^* z_{b,i} \right)^S \quad (2.6)$$

This also determines the normalisation function as $N(z) = (1 + \sum_i z_i^* z_i)^{-\frac{S}{2}}$

Matrix element of bosonic operator sequences

Consider a normal-ordered product sequence of x bosonic creation and x bosonic annihilation operators. Its matrix element for two arbitrary CSs can be shown [13] to be

$$\langle z_a | \hat{b}_{\rho_1}^\dagger \dots \hat{b}_{\rho_x}^\dagger \hat{b}_{\sigma_1} \dots \hat{b}_{\sigma_x} | z_b \rangle = z_{a,\rho_1}^* \dots z_{a,\rho_x}^* z_{b,\sigma_1} \dots z_{b,\sigma_x} \left\langle z_a^{(x)} \middle| z_b^{(x)} \right\rangle \quad (2.7)$$

where the *reduced overlap* is defined as

$$\left\langle z_a^{(x)} \middle| z_b^{(x)} \right\rangle = N(z_a)N(z_b) \left(1 + \sum_i^{M-1} z_{a,i}^* z_{b,i} \right)^{S-x} \quad (2.8)$$

i.e. the reduced unnormalised CSs behave as if their associated total particle number was reduced by x .

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

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Appendix A

Auxiliary 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