Development and application of new coherent state based methods of quantum dynamics

First Formal Progress Report

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Contents

1   Introduction

The following document is an FFPR for the post-graduate research project on coherent states the author does under the supervision of Professor Dmitry Shalashilin and Professor Orde Munro. The project aims to contribute theoretical framework for fast simulation of quantum dynamics for the COSMOS research group.

1.1   Coherent states

The task of solving the time-dependent Schrodinger equation numerically on a system with a large number of degrees of freedom M runs into the problem of time complexity, which scales exponentially with M [1, Sec. 1.2]. A possible circumvention of this problem lies in utilising a semi-classical approach, where a basis of states evolving "classically" according to the Hamiltonian is chosen, and decomposing the wavefunction into this basis allows one to study the extent of quantum coupling. Schrodinger used this idea in 1926 to formulate the "classical states" of the harmonic oscillators [2], and remarked on their useful properties: the expected values of $\hat{x}$ and $\hat{p}$ follow the classical equations of motion, and the uncertainty $\Delta x \Delta p$ does not increase in time.

Glauber, in 1963, applied the same idea to the Hamiltonian which describes the interaction between an atomic system and an electromagnetic field, forming field coherent states[1], and showed that, although not orthogonal, they form a complete basis of the Hilbert space, they minimise uncertainty, and remain coherent under time evolution [3]. Glauber constructed three equivalent definitions of field coherent states $|\alpha\rangle$ of a single mode:

- Eigenstates of the annihilation operator

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

- Minimum-uncertainty states.

- Displacements of the ground state

$$|\alpha\rangle = \exp\!\big(\alpha\hat{a}^\dagger - \alpha^*\hat{a}\big)\,|0\rangle$$

Attempting to generalise Glauber's construction to an arbitrary Hamiltonian restricts our approach. Firstly, constructing coherent states as eigenstates of the lowering operator is trivially impossible on finite-dimensional Hilbert spaces. Secondly, constructing coherent

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[1]Also known as Glauber coherent states.

states as minimum-uncertainty states is ill-advised, as it is not necessary they form a complete basis, or that unity can be resolved in them [4]. Constructing coherent states as a displacement of some reference state, however, is always possible, and a satisfactory group-theoretical formulation was found independently by Perelomov [5] and Gilmore [6] in 1972. This construction follows these steps:

1. Find the action group G of the system, i.e. a Lie group such that both the Hamiltonian and the transition operators can be expressed as functions of the elements of the Lie algebra of G.

2. Choose a reference state $|\Phi_0\rangle$ in the Hilbert space (typically the ground state or some other extremal state).

3. Find the stability subgroup $H \subset G$ which is the group of all elements of G which leave the reference state invariant up to a phase factor.

4. Find the quotient group G/H. Each element $\Omega \in G/H$ generates a unique coherent state $\Omega |\Phi_0\rangle$, and the resulting set of coherent states is topologically equivalent to the coset space G/H.

This process, as presented and discussed by Zhang, Feng, and Gilmore [7], constructs a basis of states which retain all the desired properties (coherence, minimal uncertainty, and evolution according to an effective classical Hamiltonian), and which can be constructed for a system with any dynamical group. Unity can always be resolved in this basis, which is complete but not orthogonal, and therefore overcomplete.

Moreover, if the Lie algebra of the dynamical group is semisimple, it can be transformed into the Cartan basis, where all operators in the algebra are either fully diagonal, or analogous to the creation and annihilation operators. Viscondi, Grigolo, and de Aguiar found an expression for the semiclassical propagator for such cases, which determines the overlap of two different coherent states at different times [8]. Here the full picture of the semiclassical approximation is painted: the coherent states evolve according to equations of motion governed by an effective classical Hamiltonian, and the amplitude of their overlap measures their entanglement.

1.2 Bosonic quantum dynamics

The semiclassical approach is firstly applied to bosonic systems with constant total particle number. As shown in Sec. 2, all such systems possess the same dynamical group, and thus one construction of coherent states can be used to all such systems.

The approach is applied to two particular systems:

1. The multimode Bose-Hubbard model, which is useful in description of optical lattices [9].

2. A displaced harmonic trap, which is used as a benchmark for the efficiency of the approach for a large number of modes.

The two systems have been previously studied by 1. Qiao and Grossmann [10] and 2. Green and Shalashilin [11], respectively.

Qiao and Grossmann apply a similar approach to mine in their study of the Bose-Hubbard model, constructing coherent states from the $SU(M)$ dynamical group. However, they use normalised coherent states, for which the derivation of the equations of motion is slightly different, and they do not posses some desirable properties, such as a complex quotient-space metric, due to the fact they are not analytic.

Green and Shalashilin do not use the group-theoretical $SU(M)$ coherent states. Rather, they use "coupled coherent states", which, as eigenstates of the annihilation operator, are analogous to field coherent states. These coupled coherent states are not eigenstates of the total particle number, and as such are not contained in the Hilbert space of the system, which renders them inefficient as a basis.

The aim of the first part of my project is to reproduce the results of these two investigations using analytic unnormalised $SU(M)$ coherent states based on the construction demonstrated by Viscondi, Grigolo, and de Aguiar. This would prove the efficiency and accuracy of the new group-theoretical approach to semiclassical methods, and pave the way for further work on other systems, namely fermionic quantum dynamics.

2 Theory: SU(M) coherent states

Any second-order[2] Hamiltonian for a bosonic system with M modes which preserves the total particle number can be formulated in second-quantisation in the following general form [11, p. 3]:

$$\hat{H} = \sum_{\alpha=1}^{M} \sum_{\beta=1}^{M} V_{\alpha\beta}^{(1)} \hat{a}_\alpha^\dagger \hat{a}_\beta + \frac{1}{2} \sum_{\alpha=1}^{M} \sum_{\beta=1}^{M} \sum_{\gamma=1}^{M} \sum_{\delta=1}^{M} V_{\alpha\beta\gamma\delta}^{(2)} \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\gamma \hat{a}_\delta \tag{1}$$

where $V_{\alpha\beta}^{(1)}, V_{\alpha\beta\gamma\delta}^{(2)}$ are the matrix elements of the one-body and two-body interactions, respectively.

For a total number of particles S, the Hilbert space is spanned by occupancy eigenstates

$$|s_1, s_2 \ldots s_M\rangle \quad \text{where} \quad s_1 + s_2 + \cdots + s_M = S \tag{2}$$

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[2]Comprising of one-body and two-body interactions

2.1 Quotient group G/H for bosonic systems preserving total particle number

We see that the transition operators for the occupancy basis in Eq. 2 are

$$\hat{T}_{ij} = \hat{a}_i^\dagger \hat{a}_j \tag{3}$$

and the Hamiltonian can be expressed as a second-order polynomial in terms of $\hat{T}_{ij}$. Finally, we see that

$$\left[\hat{T}_{ij}, \hat{T}_{i'j'}\right] = \hat{T}_{ij'}\delta_{i'j} - \hat{T}_{i'j}\delta_{ij'} \tag{4}$$

therefore $\hat{T}_{ij}$ forms a Lie algebra. We transform this basis like so:

$$
\begin{aligned}
\hat{S} &= \sum_{i=1}^{M} \hat{T}_{ii} \\
\hat{H}_i &= \hat{T}_{i+1,i+1} - \hat{T}_{ii} \quad \text{for} \quad i = 1, 2 \ldots M-1 \\
\hat{E}_{ij} &= \hat{T}_{ij} \quad \text{for} \quad i > j \\
\hat{E}_{ij}^\dagger &= \hat{T}_{ji} \quad \text{for} \quad i > j
\end{aligned}
$$

We see that the element $\hat{S}$ commutes with every other element, and therefore the dynamical group can be expressed as the direct product of $U(1)$ and the group generated by $\hat{H}, \hat{E}, \hat{E}^\dagger$. This second group's Lie algebra constitutes the complete matrix basis for traceless ($M \times M$) matrices, and therefore the second group is $SL(M, \mathbb{R})$. The full dynamical group is therefore $U(1) \otimes SL(M, \mathbb{R})$

We now choose a reference state. We will choose

$$|\Phi_0\rangle = |0, 0 \ldots S\rangle \tag{5}$$

This state is conventional in literature on $SU(M)$ coherent states, and is suitable for a specific reason: it is extremal in the sense that operators S, H leave it invariant up to a phase factor and operators $\hat{E}$ destroy it. Therefore we identify the general element of the quotient group G/H as

$$\hat{\Omega}(\vec{z}) = \sum_{i}^{M-1} z_i \hat{E}_{M,i}^\dagger = \sum_{i}^{M-1} z_i \hat{a}_i^\dagger \hat{a}_M \tag{6}$$

where $\vec{z}$ is an $(M-1)$-dimensional complex vector.

2.1.1 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 transition operators remain independent even if the field of coefficients is complex. Identifying the resulting operators with the generalised Gell-Mann matrices yields the dynamical group $SU(M)$ [12]. 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 [8].

Also note that the extra factor $U(1)$ in the dynamical group is commonly ignored in literature, since it is trivially included in the stability subgroup, and therefore does not affect the construction of the coherent states.

2.2 Construction and properties

Applying the quotient elements from Eq. 6 to the reference state we obtain the coherent states

$$|\vec{z}\rangle = \exp\left(\sum_i^{M-1} z_i \hat{a}_i^\dagger \hat{a}_M\right) |\Phi_0\rangle \tag{7}$$

This expression can be simplified [13] into the following form:

$$|\vec{z}\rangle = \frac{1}{\sqrt{S!}} \left(\hat{a}_M^\dagger + \sum_i^{M-1} z_i \hat{a}_i^\dagger\right)^S |0, 0 \ldots 0\rangle \tag{8}$$

Note that these states are, in general, not normalised. Therefore, I will denote unnormalized coherent states with curly brackets in the bra-ket notation, following the convention in [8], like so:

$$|\vec{z}\} = \frac{1}{\sqrt{S!}} \left(\hat{a}_M^\dagger + \sum_i^{M-1} z_i \hat{a}_i^\dagger\right)^S |0, 0 \ldots 0\rangle \tag{9}$$

The approach of Qiao and Grossmann uses a slightly different form, which imposes an extra condition to have the basis states normalised. However, this extra condition has to be accounted for in the equations of motion, which they do not do, as they expect the states to remain normalised under time evolution. This leads to overparametrisation, which is not only inefficient, but renders the construction of a quotient-space metric or identity operator in their formalism ill-formed. Viscondi, Grigolo, and de Aguiar take the unnormalized states $|z\}$ and project them onto a normalised space of equal dimension by adding a normalisation coefficient. However, since this coefficient depends on both $\vec{z}$ and $\vec{z}^*$, the normalised states are not analytic. I take a different approach: I work directly with the unnormalized states as basis vectors, and include a normalisation factor in the Lagrangian, which still permits me to use Wirtinger calculus to find the equations of motion.

2.2.1 Relationship between the coherent state and occupancy bases

By applying the multinomial theorem to Eq. 9 we obtain the decomposition of $|z\}$ into the occupancy basis:

$$|z\} = \sum_{k_1+k_1+\cdots+k_M=S} \sqrt{\frac{S!}{k_1!k_2!\ldots k_M!}} z_1^{k_1} z_2^{k_2} \ldots z_{M-1}^{k_{M-1}} |k_1, k_2 \ldots k_M\rangle \tag{10}$$

2.2.2 Overlaps and reduced forms

By applying Wick's theorem to Eq. 9 we obtain the overlap element:

$$\{\vec{z}_a | \vec{z}_b\} = (1 + \vec{z}_a^* \cdot \vec{z}_b)^S \tag{11}$$

Since unmatched creation and annihilation operators are not members of the dynamical Lie algebra, acting with them on the coherent states projects them outside of the Hilbert space. We can describe this with the reduced form of $|\vec{z}\}$, defined as follows:

$$|\vec{z}'\} = |z\} \quad \text{where} \quad S' = S - 1 \tag{12}$$

$$\left|\vec{z}^{(r)}\right\} = |z\} \quad \text{where} \quad S' = S - r \tag{13}$$

and we have

$$\hat{a}_i |\vec{z}\} = \sqrt{S} z_i |\vec{z}'\} \tag{14}$$

Therefore, the matrix element of a normal-ordered product of a set of transition operators is evaluated as follows:

$$\{\vec{z}_a | \hat{a}_{i_1}^\dagger \ldots \hat{a}_{i_r}^\dagger \hat{a}_{j_1} \ldots \hat{a}_{j_r} |\vec{z}_b\} = \begin{cases} \frac{S!}{(S-r)!} \prod_{k=1}^r z_{a,i_k}^* z_{b,j_k} \left\{\vec{z}_a^{(r)} \middle| \vec{z}_b^{(r)}\right\} & r \le S \\ 0 & r > S \end{cases} \tag{15}$$

In the above cases, we take as convention $z_M = 1$, which extends the vector without adding an extra degree of freedom, and allows for a more concise form for many equations. From this point onwards, assume this is the case in every equation unless otherwise stated.

For convenience, we will also define the reduced overlap matrix

$$X_{ab}^{(r)} = \left\{\vec{z}_a^{(r)} \middle| \vec{z}_b^{(r)}\right\} = (1 + \vec{z}_a^* \cdot \vec{z}_b)^{S-r} \tag{16}$$

2.2.3 Derivatives

Using the form in Eq. 7, we immediately see

$$\frac{\partial}{\partial z_i} |\vec{z}\} = \hat{a}_i^\dagger \hat{a}_M |\vec{z}\} \tag{17}$$

$$\frac{\partial}{\partial z_i^*} |\vec{z}\} = 0 \tag{18}$$

The time derivative can be expanded into these partial derivatives, yielding

$$\frac{\mathrm{d}}{\mathrm{d}t} |\vec{z}\} = \left(\sum_{i=1}^{M-1} \dot{z}_i \hat{a}_i^\dagger \hat{a}_M \right) |\vec{z}\} \tag{19}$$

2.2.4 Identity

Following the approach in [8], the identity operator on the quotient space is

$$\hat{I} = \int \frac{(S+M-1)!}{S! \left(1 + \vec{z}^* \cdot \vec{z}\right)^{S+M}} |\vec{z}\} \{\vec{z}| \frac{\mathrm{d}^2 \vec{z}}{\pi^{M-1}} \tag{20}$$

However, since we work with a discrete sample of the coherent states as a basis, in actuality we will use the inverse overlap matrix as an identity operator, which will allow us to decompose the initial state of the wavefunction into the basis coherent states.

2.3 Decomposition of the Schrodinger equation

Consider a (normalized) wavefunction decomposed into a basis of coherent states:

$$|\Psi(t)\rangle = \sum_{a \in \text{basis}} A_a |\vec{z}_a\} \tag{21}$$

The Lagrangian form of the Schrodinger equation is as follows[10]:

$$L(t) = \frac{\frac{i}{2} \left(\langle \Psi | \dot{\Psi} \rangle - \langle \dot{\Psi} | \Psi \rangle \right) - \langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{22}$$

However, the wavefunction is initially normalised, and, evolving according to the Schrodinger equation, it therefore remains normalised, and therefore we can omit the normalisation factor, even though we will express this Lagrangian in terms of unnormalised basis vectors.

2.3.1 Fully variational method

In the fully variational method, the time evolution of all general coordinates is coupled together.

We want to express the Lagrangian in Eq. 22 as a function of our general coordinates, which are the decomposition coefficients $A_a(t)$ and the coherent state complex elements $z_{a,i}(t)$. Applying Eq. 21 to Eq. 22 and expanding yields

$$L = \frac{i}{2} \sum_{a,b \in \text{basis}} (A_a^* \dot{A}_b - \dot{A}_a^* A_b) \{\vec{z}_a | \vec{z}_b\} + \frac{i}{2} S \sum_{a,b \in \text{basis}} A_a^* A_b \sum_{i=1}^{M-1} (z_{a,i}^* \dot{z}_{b,i} - \dot{z}_{a,i}^* z_{b,i}) \{\vec{z}_a | \vec{z}_b\}$$
$$- \sum_{a,b \in \text{basis}} A_a^* A_b \{\vec{z}_a | \hat{H} | \vec{z}_b\} \tag{23}$$

8

Applying the Euler-Lagrange equation to Eq. 23 yields the equations of motion:

$$
i \sum_{b \in \text{basis}} \dot{A}_b \left\{ \vec{z}_a | \vec{z}_b \right\} + i S \sum_{b \in \text{basis}} A_b \sum_{i=1}^{M-1} z_{a,i}^* \dot{z}_{b,i} \left\{ \vec{z}_a | \vec{z}_b \right\} = \sum_{b \in \text{basis}} A_b \left\{ \vec{z}_a | \hat{H} | \vec{z}_b \right\} \quad \text{for} \quad a \in \text{basis}
$$

(24)

$$
iSA_a^* \sum_{b \in \text{basis}} \left(\dot{A}_b z_{b,i} \left\{ \vec{z}_a' | \vec{z}_b' \right\} + A_b \dot{z}_{a,i} \left\{ \vec{z}_a | \vec{z}_b \right\} + (S-1) A_b \sum_{j=1}^{M-1} z_{a,j}^* \dot{z}_{b,j} z_{b,i} \left\{ \vec{z}_a'' | \vec{z}_b'' \right\} \right)
$$

(25)

$$
= A_a^* \sum_{b \in \text{basis}} A_b \frac{\partial}{\partial z_{a,i}^*} \left\{ \vec{z}_a | \hat{H} | \vec{z}_b \right\} \quad \text{for} \quad a \in \text{basis}, \, i = 1, 2 \ldots M - 1
$$

For a basis of size N, there are $M \cdot N$ linear equations of motion, which can be expressed in a vectorial form for the following coordinate vector:

$$
\vec{Q} = \begin{pmatrix} \vec{Q}_A \\ \vec{Q}_z \end{pmatrix}, \quad \text{where} \quad \vec{Q}_A = \begin{pmatrix} A_1 \\ \vdots \\ A_N \end{pmatrix} \quad \text{and} \quad \vec{Q}_z = \begin{pmatrix} z_{1,1} \\ z_{2,1} \\ \vdots \\ z_{N,1} \\ z_{1,2} \\ \vdots \\ z_{N,M-1} \end{pmatrix}
$$

(26)

The equations of motion are then expressable as

$$
\begin{pmatrix} X & Y \\ Y^\dagger & Z \end{pmatrix} \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \vec{Q}_A \\ \frac{\mathrm{d}}{\mathrm{d}t} \vec{Q}_z \end{pmatrix} = -i \begin{pmatrix} \vec{R}_A \\ \vec{R}_z \end{pmatrix}
$$

$$
\text{where} \quad Y_{a,Ni+b} = S z_{a,i}^* A_b X_{ab}'
$$

$$
Z_{Ni+a,Nj+b} = A_a^* A_b \left(S(S-1) X_{ab}'' z_{a,j}^* z_{b,i} + \delta_{ij} S X_{ab}' \right)
$$

$$
(R_A)_a = \sum_{b \in \text{basis}} A_b \left\{ \vec{z}_a | \hat{H} | \vec{z}_b \right\}
$$

$$
(R_z)_{Ni+a} = A_a^* \sum_{b \in \text{basis}} A_b \frac{\partial}{\partial z_{a,i}^*} \left\{ \vec{z}_a | \hat{H} | \vec{z}_b \right\}
$$

(27)

Finally, we use Eq. 1 to express $\vec{R}_A, \vec{R}_z$ using $V^{(1)}, V^{(2)}$:

$$\{\vec{z}_a|\hat{H}|\vec{z}_b\} = SX'_{ab}\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}V^{(1)}_{\alpha\beta}z^*_{a,\alpha}z_{b,\beta} + \frac{1}{2}S(S-1)X''_{ab}\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}\sum_{\gamma=1}^{M}\sum_{\delta=1}^{M}V^{(2)}_{\alpha\beta\gamma\delta}z^*_{a,\alpha}z^*_{a,\beta}z_{b,\gamma}z_{b,\delta}$$

$$\frac{\partial}{\partial z^*_{a,i}}\{\vec{z}_a|\hat{H}|\vec{z}_b\} = S(S-1)X''_{ab}z_{b,i}\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}V^{(1)}_{\alpha\beta}z^*_{a,\alpha}z_{b,\beta} + SX'_{ab}\sum_{\beta=1}^{M}V^{(1)}_{i\beta}z_{b,\beta}$$

$$+ \frac{1}{2}S(S-1)(S-2)X'''_{ab}z_{b,i}\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}\sum_{\gamma=1}^{M}\sum_{\delta=1}^{M}V^{(2)}_{\alpha\beta\gamma\delta}z^*_{a,\alpha}z^*_{a,\beta}z_{b,\gamma}z_{b,\delta} \qquad (28)$$

$$+ \frac{1}{2}S(S-1)X''_{ab}\sum_{\beta=1}^{M}\sum_{\gamma=1}^{M}\sum_{\delta=1}^{M}\left(V^{(2)}_{i\beta\gamma\delta} + V^{(2)}_{\beta i\gamma\delta}\right)z^*_{a,\beta}z_{b,\gamma}z_{b,\delta}$$

2.3.2 Decoupled basis propagation

The fully variational method is "efficient" in the sense that the coupling between the basis vectors is informed by the decomposition coefficients. However, the number of simultaneous equations is $M \cdot N$, so in each step of iteration we need to invert a square matrix with $M \cdot N$ rows, rendering the process slow. An alternative to this is to utilise one of the main properties of coherent states: they evolve along classical trajectories. The advantage is that we need to first solve N systems of $M-1$ equations, and then one system with N equations for the decomposition coefficient propagation. The disadvantage is that a basis sampled suitably for the initial conditions may not be suitable at all points in time, since the decoupled basis may "dissipate" in the quotient space, becoming too sparse. Therefore, intelligent sampling is essential for this approach.

In the decoupled basis propagation approach, we first propagate each element $|\vec{z}\}$ of our basis set. To find the equations of motion, we cannot omit the normalisation factor in the Lagrangian. There are two ways to go around is:

1. We can add a single normalisation coefficient $A(t)$ to the general coordinates, so that $|\Psi\rangle = A|\vec{z}\}$. To find the equations of motion for this coordinate system, we can use Eq. 27 with $N = 1$.

2. We can use the result from [8] for the classical trajectory of the normalised state

$$\dot{\vec{z}} = -i(g^{-1})^T\frac{\partial}{\partial\vec{z}}\frac{\{\vec{z}|\hat{H}|\vec{z}\}}{\{\vec{z}|\vec{z}\}} \quad \text{where} \quad g_{ij} = S\frac{(1+\vec{z}^*\cdot\vec{z})\delta_{ij} - z^*_i z_j}{(1+\vec{z}^*\cdot\vec{z})^2} \qquad (29)$$

Here, g_{ij} is the metric of the quotient space, as derived in Sec. 2.2.3 in [8].

After propagating every element of the basis set, we propagate the decomposition coefficients. The approach to obtain the equations of motion is analogous to Sec. 2.3.1, except we treat $z_{a,i}(t)$ as a known function. The resulting equations of motion are

$$X \dot{\vec{A}} = -i\vec{R}_A$$

$$\text{where} \quad (R_A)_a = \sum_{b \in \text{basis}} A_b \left(-iSX'_{ab} \sum_{i=1}^{M-1} z^*_{a,i} \dot{z}_{b,i} + \{\vec{z}_a | \hat{H} | \vec{z}_b\} \right) \tag{30}$$

2.4 Basis sampling

To simply go from the finite, discrete occupancy basis into the continuous, overcomplete, non-orthogonal basis of coherent states would surely not help if we wanted to use the entire quotient space as our basis. Relying on the semi-classical approximation, we shall instead sample a small discrete subset of the quotient space and use the equations of motion derived in Sec. 2.3.1 and Sec. 2.3.2. Therefore the efficiency and accuracy of our results will depend strongly on the method of sampling.

Typically, our initial wavefunction will be a pure coherent state, which will be chosen as the first element of the basis set. However, even if this is the case, we cannot set $A_a(t = 0) = \delta_{a,1}$, since the matrix $\begin{pmatrix} X & Y \\ Y^\dagger & Z \end{pmatrix}$ will not be invertible. Instead, we will utilise the non-orthogonality of the basis set, applying the identity operator to find the initial decomposition coefficients. The continuous identity operator in Eq. 20 is not helpful, so we use the inverse overlap matrix operator defined as follows [8, Eq. 13]:

$$\hat{I}_X = \sum_{a \in \text{basis}} \sum_{b \in \text{basis}} |\vec{z}_a\} (X^{-1})_{ab} \{\vec{z}_b| \tag{31}$$

Because of the finite size of the basis, it may be necessary to renormalise the wavefunction after applying this identity operator to assure $\langle \Psi | \Psi \rangle = 1$.

2.4.1 Conditioning

For each finite step of the numerical integration, the step size is uniform for each element of the coordinate vector $\vec{Q}$, even though this step size will be different for different steps. A sane algorithm for numerical integration (such as the Dormand-Prince method used so far in the project) will estimate the step size based on the maximum allowed error obtained in the step and the value of the coordinate time derivative $\dot{\vec{Q}}$. However, should a subset of elements of this time derivative be much larger than its complement, it will severely limit the step size, and the algorithm becomes inefficient for a large number of coordinates, performing

needlessly small steps. To conteract this, we will condition the initial overlap matrix by limiting the fraction of its maximal and minimal eigenvalue

$$\frac{\lambda_{\max}}{\lambda_{\min}} < \epsilon_{\lim} \tag{32}$$

I chose a simple algorithm described in [14]. A weight function is chosen as a gaussian centered around the initial state $\vec{z}_0$. Candidate basis vectors are drawn from the full quotient space according to the weight function and added to the basis only if their addition does not violate the conditioning limit in Eq. 32. The process terminates either if the desired basis size is reached, or if a certain number of candidates are discarded in a row, resulting in a saturated basis.

2.5   Regularisation

The process of solving the equations of motion is built upon inverting some matrix M which acts on $\dot{\vec{Q}}$. Therefore, the numerical stability of the integration process is dependent on the values of eigenvalues of M. If these eigenvalues become too small, a finite step may cause a large, unphysical change in $\vec{Q}$, which sabotages the accuracy of the solution. To counteract this, we regularise the matrix M by adding τI, i.e. some value τ to every element on the diagonal, utilising the fact that the sum of eigenvalues of M equals $\operatorname{Tr} M$, which lowers the probability of the eigenvalues of M^{-1} diverging. τ, the regular timescale, has to be chosen small enough to not affect the equations of motion on well-behaved regimes.

3   Progress and outlook

3.1   Provisional results

3.2   Next steps in research

better numerical resolution
  better stability
  how about using the semiclassical propagator to make the basis sampling ULTRA clever
  fermions lessgooo
  ZOMBIE STATES???? reference pls :))) lit af

3.3 Training plan

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