Coupled Coherent States for Indistinguishable Bosons in the Second Quantisation Representation

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Computer simulations of many-body quantum dynamics of indistinguishable particles is a challenging task for computational physics. In this paper we demonstrate that the method of coupled coherent states (CCS) developed previously for multidimensional quantum dynamics can be used to study indistinguishable bosons in the second quantisation formalism. To prove its validity, the technique termed here coupled coherent states for indistinguishable bosons (CCSB) is tested on two model problems. The first is a system-bath problem consisting of a tunnelling mode coupled to a harmonic bath, previously studied by CCS and other methods in distinguishable representation in 20 dimensions. The harmonic bath is comprised of identical oscillators, and may be second quantised for use with CCSB. The cross-correlation function for the dynamics of the system and Fourier transform spectrum compare extremely well with a benchmark calculation, and are in much better agreement than prior methods of studying the problem. The second model problem involves 100 bosons in a shifted harmonic trap. Oscillations in the 1-body density are calculated and shown to compare favourably to a multiconfigurational time-dependent Hartree for bosons calculation, demonstrating the applicability of the method as a new formally exact way to study the quantum dynamics of Bose-Einstein condensates.

INTRODUCTION

In the past two decades there has been significant interest in systems of indistinguishable bosons, due to experimentally produced Bose-Einstein condensates of ultracold alkali metal atoms [1–3]. These condensates, first posited by the eponymous Bose and Einstein in 1924-25, have permitted macroscopic observations of quantum phenomena and lead to a wealth of experimental research in areas such as atomic interferometry [4], bosonic Josephson junctions [5, 6] and quantum vortices [7, 8].

From the theoretician’s point of view, the Gross-Pitaevski equation (GPE) [9, 10] has been the predominant method used to study Bose-Einstein condensates, see for example Refs. [11–16] and the review articles [17, 18]. However the GPE is a mean-field theory and as such cannot describe many-body effects in condensates. It also assumes that all bosons occupy a single state at all times, which is not the case during fragmentation. In recent years, the multiconfigurational time-dependent Hartree method for bosons (MCTDHB) [19, 20], and its extension to multilayer formalism (ML-MCTDHB) [21] have been used to treat indistinguishable bosons from the standpoint of exact quantum mechanics (see Refs. [22–32] and [33–36] for applications of MCTDHB and ML-MCTDHB respectively).

Before being used to treat indistinguishable bosons, standard MCTDH [37] and ML-MCTDH [38, 39] have been well established theories for treating distinguishable particles. They are able to solve the time-dependent Schrödinger equation (TDSE) exactly for multiple degrees of freedom, albeit with basis sets that grow exponentially with increased dimensionality. Our own coupled coherent states (CCS) method has also demonstrated its propensity at solving the TDSE for distinguishable particles, with basis sets that scale more favourably with dimensionality [40, 41]. This is achieved by using randomly sampled trajectory guided coherent states as basis functions, although the trade-off for this favourable scaling is that random noise and slow convergence may be present.

In this present work we extend the CCS method to looking at indistinguishable bosons in the second quantisation representation, and dub the method coupled coherent states for indistinguishable bosons (CCSB). Due to the use of coherent states in CCSB and their relation to the creation and annihilation operators of second quantisation, together with the fact that systems with a large number of particles tend towards classical behaviour and the basis in CCS is guided by classical-like trajectories, suggest that the method will be particularly suited to such systems. Indeed, recent semiclassical coherent state work on indistinguishable bosons demonstrates this hypothesis [42, 43]. To illustrate the suitability of CCSB, we apply the method to two model problems. The CCSB method provides a new exact way of treating systems of indistinguishable bosons, and the aim of the method is to be used to study Bose-Einstein condensate systems.

NUMERICAL DETAILS

The CCS formalism represents the wavefunction by a trajectory guided basis set of frozen Gaussians, or equivalently coherent states, $|z\rangle$ coupled to fully quantum amplitudes. This has been derived and presented previously when treating distinguishable particles [40, 41], and the wavefunction representation and relevant working equations are shown in the Appendix. No modification of the working equations is required for treating indistin-
guishable bosons with CCSB, however, the coherent state basis functions are used to represent particle number occupations of quantum states in the second quantisation formalism, as opposed to individual particles in the distinguishable first quantisation representation.

In the second quantisation representation, multiparticle states are described in terms of an occupation number \( n^{(a)} \) that describes the number of particles belonging to a particular quantum state \( |a\rangle \). A Fock state describes the set of occupation number states

\[
|n\rangle = \prod_{a=0}^{\Omega} |n^{(a)}\rangle = |n^{(0)}, n^{(1)}, \ldots, n^{(\Omega)}\rangle, \quad (1)
\]

and may be generated by successive application of creation operators on the vacuum state \( |0\rangle \)

\[
|n^{(0)}, n^{(1)}, \ldots, n^{(\Omega)}\rangle = \frac{(\hat{a}^{(0)})^{n^{(0)}}}{\sqrt{n^{(0)}!}} \frac{(\hat{a}^{(1)})^{n^{(1)}}}{\sqrt{n^{(1)}!}} \cdots \frac{(\hat{a}^{(\Omega)})^{n^{(\Omega)}}}{\sqrt{n^{(\Omega)}!}} |0^{(0)}, 0^{(1)}, \ldots, 0^{(\Omega)}\rangle. \quad (2)
\]

In CCSB, the multidimensional version of the CCS wavefunction representation is used as a basis set expansion for Fock states

\[
|n\rangle = \sum_{k=1}^{K} D_k(t)e^{iS_k(t)} |z_k(t)\rangle, \quad (3)
\]

where the sum is over \( K \) configurations, \( D_k \) is a quantum amplitude propagated via the time-dependent Schrödinger equation, \( S_k \) is the classical action, and \( |z_k\rangle \) is a coherent state guided by classical trajectories, with

\[
|z_k\rangle = \prod_{a=0}^{\Omega} |z^{(a)}\rangle. \quad (4)
\]

The multidimensional coherent state \( |z_k\rangle \) is a product of coherent states that describe occupations of each quantum state \( |a\rangle \). Therefore any wavefunction in the basis of Fock states can be equivalently represented in the basis of coherent states. The Hamiltonian of a system of indistinguishable bosons can be second quantised and presented in terms of 1-body \( \hat{h}(Q) \), 2-body \( \hat{W}(Q, Q') \), and creation and annihilation operators as

\[
\hat{H} = \sum_{a,\beta} \langle a|\hat{h}|\beta\rangle \hat{a}^{(a)\dagger} \hat{a}^{(\beta)} + \frac{1}{2} \sum_{a,\beta,\gamma,\zeta} \langle a,\beta|\hat{W}|\gamma,\zeta\rangle \hat{a}^{(a)\dagger} \hat{a}^{(\beta)\dagger} \hat{a}^{(\gamma)} \hat{a}^{(\zeta)}, \quad (5)
\]

where \( |a\rangle, |\beta\rangle, |\gamma\rangle, \) and \( |\zeta\rangle \) are quantum states. This conveniently gives a second quantised Hamiltonian in normal ordered form, which is required by CCSB. In the following sections CCSB is applied to two model problems.

**APPLICATION 1: DOUBLE WELL TUNNELLING PROBLEM**

The first application of CCSB is to an \( M \)-dimensional model Hamiltonian that consists of an \((M - 1)\)-dimensional harmonic bath, coupled to a 1-dimensional tunnelling mode governed by an asymmetric double well potential. This a system-bath problem previously studied in distinguishable representation by: matching pursuit split-operator Fourier transform (MP/SOFT) [44], standard CCS [45], a trajectory guided configuration interaction (CI) expansion of the wavefunction [46], a 2-layer version of CCS (2L-CCS) [47], and an adaptive trajectory guided (aTG) scheme [48]. A benchmark calculation has also been proposed in recent work [49], using a relatively simple wavefunction expansion in terms of particle in a box wavefunctions for the tunnelling mode, and harmonic oscillator wavefunctions for the harmonic bath. The size of the calculation was greatly reduced by exploiting the indistinguishability of the bath configurations, the first time this had been considered, and a well converged result was achieved, prompting the idea of CCSB. The Hamiltonian is given in distinguishable representation by

\[
\hat{H} = \frac{\hat{q}^{(1)2}}{2} - \frac{\hat{q}^{(1)4}}{2} + \frac{\hat{q}^{(1)4}}{16\eta} + \hat{P}^2 + \frac{(1 + \lambda\hat{q}^{(1)})^2}{2} \quad (6)
\]

where \( \hat{q}^{(1)}, \hat{p}^{(1)} \) are the position and momentum operators of the 1-dimensional system tunnelling mode, and \( (Q, P) \) are the position and momentum operators of the \((M - 1)\)-dimensional harmonic bath modes, with \( Q = \sum_{m=2}^{M} \hat{q}^{(m)} \) and \( P = \sum_{m=2}^{M} \hat{p}^{(m)} \). The coupling between system and bath is given by the constant \( \lambda \) whilst \( \eta \) determines the well depth.

In previous work [44–49], the parameters \( \lambda = 0.1 \) and \( \eta = 1.3544 \) have been used in a 20-dimensional \((M = 20)\) problem, which we also consider. The initial wavefunction \( |\Psi(0)\rangle \) is a multidimensional Gaussian wavepacket, with initial position and momentum centres for the tunnelling mode \( \hat{q}^{(1)}(0) = -2.5 \) and \( \hat{p}^{(1)}(0) = 0.0 \), and for the bath modes \( \hat{q}^{(m)}(0) = 0.0 \) and \( \hat{p}^{(m)}(0) = 0.0 \) \forall \( m \).

As the bath oscillators have the same initial conditions and the same frequency, they can be thought of as indistinguishable, and the bath part of the Hamiltonian may be second quantised for use with CCSB. As the tunnelling mode is not part of this indistinguishable system, the portion of the Hamiltonian that describes it will not be second quantised. However, this will not pose a problem as the dynamical equations are identical for CCS and CCSB, the only subtlety is the interpretation of the coherent state basis vectors \( |z\rangle \) as will be discussed below. Using the definition of a second quantised Hamiltonian in Eq. 5, and the definition of coherent states as eigenstates of the creation and annihilation operators, it may be written in normal-ordered form as
where the quantum states $|\alpha\rangle$ and $|\beta\rangle$ are those of the harmonic oscillator with $\alpha$ and $\beta$ numbers of quanta, $\epsilon^{(\alpha)}$ is the eigenvalue for $|\alpha\rangle$, and the position and momentum operators of the tunneling mode have explicitly been labelled with $(m = 1)$ to distinguish them from the $\alpha$ labelling scheme of the second quantised bath modes. A full derivation of this, alongside evaluation of the $Q^{(2\alpha, 2\beta)}$ matrix element is shown in the Appendix. Note that only even harmonic oscillator levels are required due to all bath modes initially residing in the ground level, and the Hamiltonian having quadratic coupling to the system meaning only even harmonic oscillator levels will be occupied.

The multidimensional coherent state basis vector $|z\rangle$ is represented as

$$|z\rangle = |z^{(m=1)}\rangle \prod_{\alpha=0}^{\Omega} |z^{(2\alpha)}\rangle$$

where $|z^{(m=1)}\rangle$ is a basis function for the tunneling mode and $|z^{(2\alpha)}\rangle$ is a basis function for the second quantised bath modes. The determination of initial conditions for these coherent state basis functions, as well as the values of the initial amplitudes is shown in the Appendix.

The quantity of interest used to assess the performance of CCSB and compare it to previous methods of studying the problem [44–49] is the cross-correlation function (CCF). This is the overlap between the wavefunction at time $t$ and the mirror image of the initial wavepacket, $|\bar{\Psi}(0)\rangle$, i.e. $\langle \bar{\Psi}(0)|\Psi(t)\rangle$. The mirror image of the initial state has coordinates for the tunneling mode of $\bar{q}^{(1)}(0) = +2.5$ and $\bar{p}^{(1)}(0) = 0.0$, with bath modes in the ground harmonic level. It is located in the upper well of the asymmetric double well tunneling potential, therefore non-zero values of the CCF are indicative of tunneling. The spectrum of the CCF is also presented via a Fourier transform (FT) of the real part of the CCF.

The results of the CCSB calculation compared with previous methods of studying the 20D, $\lambda = 0.1$ case [44–49] is shown in Fig. 1 with CCFs on the left hand side of the figure, and FT spectra on the right hand side. The CCSB calculation uses $K = 4000$ configurations and $\Omega = 5$ even harmonic oscillator levels in the bath basis. The dimensionality of this problem has therefore been reduced from 20 to 6.

As can be seen from these two figures, the CCSB results compare extremely favourably to the benchmark calculation, with much closer agreement than prior methods. Previously the trajectory guided CI expansion was the closest result to the benchmark, due to its basis set expansion of time-independent basis functions used to represent excited state configurations being similar to the benchmark approach. However the CCF still differed from the benchmark, possibly due to approximations used in sampling the potential energy surface, despite the FT obtaining splitting of the higher energy peaks that no prior method managed. For this present CCSB calculation, there is no significant degradation of the calculation at $t > 25$ a.u. as with the other methods, and the splitting of the high energy peaks is very well reproduced. As was alluded to in Ref. [47], for this Hamiltonian a detailed description of the bath is required for accurate propagation, which is achieved in CCSB by taking account of the symmetry of the Hamiltonian.

APPLICATION 2: INDISTINGUISHABLE BOSONS IN A DISPLACED HARMONIC TRAP

The second application of CCSB is to a system composed purely of indistinguishable bosons, with $N$ weakly interacting bosons placed in a harmonic trap displaced from the origin. The oscillations in the density are calculated and compared to an MCTDHB [19, 20] result with 1 orbital (calculated by the authors, using the MCTDHB package [50]) that is equivalent to the Gross-Pitaevskii equation. However, unlike the Gross-Pitaevskii equation, CCSB is not a mean-field approach but a fully quantum technique like MCTDHB.

The Hamiltonian (in dimensionless units and distinguished representation) for this problem consists of a shifted harmonic potential and a 2-body interaction term

$$\hat{H} = \frac{\hat{P}^2}{2} + \frac{(\hat{Q} - \xi)^2}{2} + \hat{W}(\hat{Q}, \hat{Q}').$$

where $\hat{Q}$ and $\hat{P}$ are the position and momentum operators of the $N$ bosons, $\xi = 2.1$ is a parameter that shifts the harmonic potential from the origin, and $\hat{W}$ is the 2-body interaction, given by the contact interaction

$$\hat{W}(\hat{Q}, \hat{Q}') = \lambda_0 \delta(\hat{Q} - \hat{Q}').$$

The constant $\lambda_0 = 0.001$ indicates weak interactions and accounts for the mean-field effects in MCTDHB with 1
FIG. 1: Comparison of cross-correlation functions (left, real parts in black and absolute values in red) and Fourier transforms of the real part of the cross-correlation functions (right) for different methods of studying Eq. 6 with $M = 20$, $\lambda = 0.1$ parameters: (a) MP/SOFT [44], (b) Trajectory Guided CI Expansion [46], (c) aTG [48], (d) CCS [45], (e) 2L-CCS [47], (f) CCSB (present work), (g) Benchmark [49].
FIG. 2: Space-time representation of the evolution of the 1-body density for (a) MCTDHB with 1 orbital and (b) CCSB with \( K = 250 \) configurations and \( \Omega = 25 \) harmonic oscillator levels in the basis.

The derivation of the above, and evaluation of the matrix elements \( Q^{(\alpha,\beta)} \) and \( \delta^{(\alpha,\beta,\gamma,\zeta)} \) is shown in the Appendix. For this problem \( N = 100 \) bosons in the trap are used, where all reside in the ground harmonic oscillator state initially. The initial sampling of the coherent states and amplitudes is shown in the Appendix.

The dynamics are followed by observing the evolution of the density matrix over the course of the calculation, which in CCSB can be evaluated by the following

\[
\rho(Q) = \langle \alpha | \rho^{(\alpha,\beta)} | \beta \rangle = \sum_{\alpha,\beta=0}^{\Omega} \frac{1}{2^{\alpha} \alpha!} \frac{1}{\sqrt{2^{\beta} \beta!}} \left( \frac{1}{\pi} \right)^{1/4} e^{-Q^2/2H_{\alpha}(Q)}\rho^{(\alpha,\beta)} \times \left( \frac{1}{\pi} \right)^{1/4} e^{-Q^2/2H_{\beta}(Q)}.
\]

(13)

This 1-body density is shown as a function of position and time for CCSB and MCTDHB in Fig. 2. The CCS calculation uses \( K = 250 \) configurations and \( \Omega = 25 \) harmonic oscillator levels in the basis. It can be seen from the figures that CCSB compares well with the MCTDHB calculation, reproducing the oscillation in the 1-body density of the bosonic cloud due to the displacement of the potential from the origin. This brief initial application to a Bose-Einstein condensate system provides impetus for investigation of further problems in this vein with CCSB.
CONCLUSIONS

In this work the CCS method has been straightforwardly applied to investigation of indistinguishable bosons, as MCTDH and ML-MCTDH have been, and the method dubbed CCSB. Instead of the coherent state basis functions being used to represent individual particles like in the standard distinguishable representation of CCS, in CCSB they are used as a basis for number occupation of quantum states in the second quantisation Fock state formalism.

Two example model Hamiltonians have been studied, demonstrating the accuracy of the method. In the first example, CCSB was applied to the system-bath asymmetric double well tunnelling problem previously studied in Refs. [44–49] in distinguishable representation. As the bath is comprised of oscillators of the same frequency, they were treated as indistinguishable and the bath portion of the Hamiltonian second quantised. The system tunnelling portion of the Hamiltonian was kept in distinguishable representation, therefore this first application was a hybrid of standard CCS and CCSB. This does not pose a problem however, as the working equations for trajectories and time-dependence of amplitudes are the same in each. The previously studied 20D, system-bath coupling \( \lambda = 0.1 \) case [44–49] was investigated, and the second quantised bath required \( \Omega = 5 \) harmonic oscillator levels in the basis for the converged result, thus the dimensionality of the problem was reduced from 20 to 6. The CCSB calculation was in much better agreement with a benchmark result [49] on the system than all other methods that have studied the problem.

In the second example, a model Hamiltonian for a system of 100 bosons in a shifted harmonic trap was studied, and oscillations in the 1-body density calculated. This is a system composed entirely of indistinguishable bosons, and provided an introductory test for CCSB in the realm of Bose-Einstein condensates. Ultimately, the method is aimed for use in studying such systems. Matrix elements of 2-body operators had to be calculated, as is common for interacting condensates, and these may be computed analytically by CCSB. The density oscillations were compared to a MCTDHB [19, 20] calculation that was equivalent to using the Gross-Pitaevskii equation [9, 10], which are two of the main methods used for studying condensates theoretically. The CCSB result compared well to that of MCTDHB/GPE, and provides motivation for further study on more challenging Bose-Einstein condensate systems. Finally, it is important to reiterate that CCSB is not a mean-field approach, but a formally exact method for the solution of the time-dependent Schrödinger equation like MCTDHB.

Future avenues of research for CCSB include more complicated Bose-Einstein condensate problems, such as the combination of the method with one to treat identical fermions [52] to study Bose-Fermi mixtures, as has been carried out by MCTDH [53] and ML-MCTDH [54]; and incorporation of SU(n) coherent states, as demonstrated in Ref. [55].

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In the CCS method, the wavefunction is represented as a basis set of trajectory guided coherent states, $|z\rangle$. The coordinate representation of a coherent state is given by

$$\langle x|z \rangle = \left(\frac{-\gamma}{\pi}\right)^{1/4} \exp\left(-\frac{\gamma}{2}(x-q)^2 + \frac{i}{\hbar}p(x-q) + \frac{ipq}{2\hbar}\right),$$

(14)

where $q$ and $p$ are the position and momentum centres of the coherent state, $\gamma$ is the width parameter of the coherent state, given by $\gamma = m\omega/\hbar$, with $m$ the mass and $\omega$ the frequency. In atomic units (which will be used throughout the remainder of the paper) $m = \omega = \hbar = 1$, thus $\gamma = 1$. Coherent states are eigenstates of the creation and annihilation operators respectively

$$\langle z|\hat{a}^\dagger = \langle z| z^*$$
$$\hat{a}|z\rangle = z|z\rangle,$$

(15a)

(15b)

where the creation and annihilation operators are given by

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}} (\hat{q} - i\hat{p})$$
$$\hat{a} = \frac{1}{\sqrt{2}} (\hat{q} + i\hat{p}).$$

(16a)

(16b)

The eigenvalues of Eqs. 15a and 15b, $z$ and $z^*$, can be used to label a coherent state, and from Eqs. 16a and 16b it can be seen they are given by

$$z = \frac{1}{\sqrt{2}} (q + ip)$$
$$z^* = \frac{1}{\sqrt{2}} (q - ip).$$

(17a)

(17b)

An important consequence of the above is that one may write a Hamiltonian in terms of creation and annihilation operators rather than position and momentum operators. A normal ordered Hamiltonian may then be obtained when the creation operators precede the annihilation ones

$$\hat{H}(\hat{q},\hat{p}) = \hat{H}(\hat{a},\hat{a}^\dagger) = H_{\text{ord}}(\hat{a}^\dagger, \hat{a}).$$

(18)

From this, matrix elements of the Hamiltonian are simple to calculate in a coherent state basis

$$\langle z'|H_{\text{ord}}(\hat{a}^\dagger, \hat{a})|z\rangle = \langle z'|z\rangle H_{\text{ord}}(z^*, z),$$

(19)

where the overlap $\langle z'|z\rangle$ is given by

$$\langle z'|z\rangle = \exp\left(z^*z - \frac{z^*z'}{2} - \frac{z^*z}{2}\right).$$

(20)

The wavefunction ansatz in CCS is given by

$$|\Psi(t)\rangle = \sum_{k=1}^{K} D_k(t)e^{iS_k(t)}|z_k(t)\rangle,$$

(21)

where the sum is over $K$ configurations, $D_k$ is a time dependent amplitude and $S_k$ is the classical action. The classical action in coherent state notation is given by

$$S_k = \int \left[\frac{i}{2} (z_k^*\dot{z}_k - \dot{z}_k^*z_k) - H_{\text{ord}}(z_k^*, z_k)\right] dt.$$
The wavefunction is propagated via the time-dependence of the coherent state basis vectors, amplitudes and action. The coherent states are guided by classical trajectories, and evolve according to Hamilton’s equation

$$\dot{z}_k = -i \frac{\partial H_{\text{ord}}(z_k^*, z_k)}{\partial z_k^*}. \quad (23)$$

The time-dependence of the amplitudes may be found via substitution of Eq. 21 into the time-dependent Schrödinger equation and closing with a coherent state basis bra:

$$\sum_{i=1}^{K} (z_k | z_i) e^{i S_i} \frac{d D_i}{dt} = -i \sum_{i=1}^{K} (z_k | z_i) e^{i S_i} D_i \delta^2 H_{\text{ord}}(z_k^*, z_i), \quad (24)$$

where the $\delta^2 H_{\text{ord}}(z_k^*, z_i)$ term is

$$\delta^2 H_{\text{ord}}(z_k^*, z_i) = H_{\text{ord}}(z_k^*, z_i) - H_{\text{ord}}(z_i^*, z_i) - i \dot{z}_i (z_k^* - z_i^*). \quad (25)$$

Finally, the time-dependence of the classical action is straightforwardly calculated from Eq. 22.

**Second Quantisation of Hamiltonian for Application 1**

Using the definition of a second quantised Hamiltonian in Eq. 5 in the main text, Eq. 6 may be written as

$$\hat{H} = \frac{\hat{p}^2(\alpha=1)^2}{2} - \frac{\hat{q}^2(\alpha=1)^2}{2} + \frac{\hat{q}^2(\alpha=1)^4}{16 \eta} + \left[ \sum_{\alpha, \beta=0}^{\Omega} \langle \alpha | \hat{P}^2_2 + \hat{Q}^2_2 | \beta \rangle \hat{a}^{\dagger} \hat{a}^{\dagger} \right] + \frac{\lambda \hat{q}^2(\alpha=1)}{2} \left[ \sum_{\alpha, \beta=0}^{\Omega} Q(\alpha, \beta) \hat{a}^{\dagger} \hat{a}^{\dagger} \right] \quad (26)$$

The quantum states $|\alpha\rangle$ and $|\beta\rangle$ are those of the harmonic oscillator with $\alpha$ and $\beta$ numbers of quanta, and the equality on the second line for $(\alpha | \hat{P}^2_2 + \hat{Q}^2_2 | \beta)$ follows because this is non-zero with eigenvalue $e^{\alpha}$ only when $\alpha = \beta$. The sums are from the ground level $\alpha = 0$, to some upper level $\Omega$. In principle, one should choose $\Omega = \infty$ for a complete description of the bath, however in practice additional oscillator levels may simply be added on until a converged result is achieved. The position and momentum operators of the tunnelling mode have explicitly been labelled with $(m = 1)$ to distinguish them from the $\alpha$ labelling scheme of the second quantised bath modes.

The matrix $Q(\alpha, \beta)^2$ is evaluated as

$$\langle \alpha | \hat{Q}^2_2 | \beta \rangle = \begin{cases} \frac{1}{2} \sqrt{(\alpha + 2)(\alpha + 1)} & \text{if } \alpha = \beta - 2 \\ \frac{1}{2} \sqrt{\alpha(\alpha - 1)} & \text{if } \alpha = \beta + 2 \\ e^{\alpha} & \text{if } \alpha = \beta \\ 0 & \text{otherwise.} \end{cases} \quad (27)$$

As this matrix is non-zero only for quanta $\alpha = \beta$ and $\alpha = \beta \pm 2$, and we may say that all bath modes are initially in the ground harmonic oscillator level ($\alpha = 0$) as they are at the origin in distinguishable representation (previously assumed in the benchmark calculation [49]), only harmonic oscillator levels with even numbers of quanta will be included and the bottom line of Eq. 26 is written as

$$\hat{H} = \frac{\hat{p}^2(\alpha=1)^2}{2} - \frac{\hat{q}^2(\alpha=1)^2}{2} + \frac{\hat{q}^2(\alpha=1)^4}{16 \eta} + \left[ \sum_{\alpha=0}^{\Omega} e^{2(\alpha)} \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a} \right] + \frac{\lambda \hat{q}^2(\alpha=1)}{2} \left[ \sum_{\alpha, \beta=0}^{\Omega} Q(2\alpha, 2\beta)^2 \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a} \right]. \quad (28)$$
Initial Conditions for Application 1

The initial coherent state basis functions for the tunnelling mode are sampled from a Gaussian distribution centered around the initial tunnelling mode coordinates and momenta, as in previous works \cite{45, 47}

\[
f(z^{(m=1)}) \propto \exp \left( -\sigma^{(m=1)} \left| z^{(m=1)} - z^{(m=1)}(0) \right|^2 \right),
\]

where \(\sigma^{(m=1)}\) is a parameter governing the width of the distribution.

Sampling the initial coherent states for the bath can be performed by obtaining a probability distribution from the square of the coherent state representation of the initial bath Fock state. The initial bath Fock state is equal to

\[
|n\rangle = \prod_{\alpha=0}^{\Omega} |n^{(2\alpha)}\rangle = |n^{(2\alpha=0)}, n^{(2\alpha=2)}, \ldots, n^{(2\alpha=2\Omega)}\rangle = |(M-1), 0, \ldots, 0\rangle,
\]

where there are \(M-1\) bath oscillators all in the ground harmonic oscillator state. Using the representation of a coherent state in a basis of Fock states

\[
|z\rangle = e^{-\frac{|z|^2}{4}} \sum_{\alpha} \frac{z^{n^{(\alpha)}}}{\sqrt{n^{(\alpha)!}}} |n^{(\alpha)}\rangle
\]

the following may be obtained

\[
|\langle z^{(2\alpha)}|n^{(2\alpha)}\rangle|^2 = \frac{e^{-|z^{(2\alpha)}|^2} \left(|z^{(2\alpha)}|^2\right)^{n^{(2\alpha)}}}{\pi \Gamma(2\alpha+1)},
\]

where the value of \(\pi\) has appeared to enforce normalisation. This resembles a Poissonian distribution, however \(|z^{(2\alpha)}|^2\) is continuous so a gamma distribution is used instead

\[
f(|z^{(2\alpha)}|^2) \propto \frac{(|z^{(2\alpha)}|^2)^{n^{(2\alpha)}} e^{-|z^{(2\alpha)}|^2}}{\Gamma(n^{(2\alpha)}+1) (\sigma^{(2\alpha)})^{n^{(2\alpha)+1}}},
\]

where \(\sigma^{(2\alpha)}\) is a compression parameter controlling the width of the distribution, and \(\Gamma\) is the gamma function that is calculated using \(n^{(2\alpha)} + 1\) because \(\Gamma(n) = (n-1)!\).

The gamma distribution will be centred around \(\sigma^{(2\alpha)} n^{(2\alpha)}\), however \(|\langle z^{(2\alpha)}|n^{(2\alpha)}\rangle|^2\) should be centred around \(|z^{(2\alpha)}|^2 = n^{(2\alpha)}\) as its maximum is found by

\[
\frac{\text{d}}{\text{d}|z^{(2\alpha)}|^2} \langle z^{(2\alpha)}|n^{(2\alpha)}\rangle^2 = \frac{1}{\pi \Gamma(2\alpha)!} \left( -e^{-|z^{(2\alpha)}|^2} \left(|z^{(2\alpha)}|^2\right)^{n^{(2\alpha)}} + n^{(2\alpha)} e^{-|z^{(2\alpha)}|^2} \left(|z^{(2\alpha)}|^2\right)^{n^{(2\alpha)+1}} - 1 \right) = 0.
\]

Fortunately, this is not an issue, as when \(n^{(2\alpha)} = 0\) the distribution will be centred around 0 irrespective of the compression parameter, and for \(n^{(2\alpha=0)} = M-1\) a compression parameter of \(\sigma^{(2\alpha=0)} = 1.0\) is used. In the \(M = 20\) case in the main text, the compression parameter for all occupation states with \(n^{(2\alpha)} = 0\) is \(\sigma^{(2\alpha>0)} = 100\).

The initial amplitudes are calculated by projection of the initial basis onto the initial wavefunction with the action set to zero

\[
\langle z_k(0)|\Psi(0)\rangle = \sum_{l=1}^{K} D_l(0) \langle z_k(0)|z_l(0)\rangle.
\]

The overlap of the initial coherent state basis with the initial wavefunction can be decomposed to

\[
\langle z_k(0)|\Psi(0)\rangle = \langle z_k^{(m=1)}(0)|\Psi^{(m=1)}(0)\rangle \prod_{\alpha=0}^{\Omega} \langle z_k^{(2\alpha)}(0)|n\rangle.
\]
The coherent state overlap with initial bath Fock state can be calculated by once more using the coherent state representation in a basis of Fock states, Eq. 31. The overlap with the unoccupied states will be equal to 1, therefore only the ground harmonic oscillator state with occupation $n^{(2\alpha=0)} = M - 1$ will contribute

$$
\langle \prod_{\alpha=0}^{\Omega} z_k^{(2\alpha)}(0)|n^{(2\alpha=0)}\rangle = \langle z_k^{(2\alpha=0)}(0)|n^{(2\alpha=0)}\rangle
$$

$$
e^{-\frac{\langle z_k^{(2\alpha=0)}(0)\rangle^{2}}{2}} \langle z_k^{(2\alpha=0)}(0)\rangle^{M-1} \sqrt{(M-1)!}.
$$

Second Quantisation of Hamiltonian for Application 2

Using the definition of a second quantised Hamiltonian in Eq.5 in the main text, Eq. 9 may be written as

$$
\hat{H} = \sum_{\alpha, \beta=0}^{\Omega} \langle \alpha | \hat{p}^2 | \beta \rangle \hat{a}^{(\alpha)\dagger} \hat{a}^{(\beta)} - \sum_{\alpha, \beta=0}^{\Omega} \langle \alpha | \xi \hat{Q} | \beta \rangle \hat{a}^{(\alpha)\dagger} \hat{a}^{(\beta)} + \sum_{\alpha, \beta=0}^{\Omega} \langle \alpha | \xi \hat{Q} | \beta \rangle \hat{a}^{(\alpha)\dagger} \hat{a}^{(\beta)} + \sum_{\alpha=0}^{\Omega} \langle \alpha | \hat{p}^2 | \alpha \rangle \hat{a}^{(\alpha)\dagger} \hat{a}^{(\alpha)}
$$

$$
+ \frac{1}{2} \sum_{\alpha, \beta, \gamma, \zeta=0}^{\Omega} \langle \alpha, \beta|\lambda_0 \delta(\hat{Q} - \hat{Q}')|\gamma, \zeta\rangle \hat{a}^{(\alpha)\dagger} \hat{a}^{(\beta)} \hat{a}^{(\gamma)\dagger} \hat{a}^{(\zeta)\dagger}
$$

$$
= \sum_{\alpha=0}^{\Omega} \epsilon^{(\alpha)} \hat{a}^{(\alpha)\dagger} \hat{a}^{(\alpha)} - \sum_{\alpha, \beta=0}^{\Omega} \xi \hat{Q}^{(\alpha, \beta)} \hat{a}^{(\alpha)\dagger} \hat{a}^{(\beta)} + \sum_{\alpha=0}^{\Omega} \frac{\xi^2}{2} \hat{a}^{(\alpha)\dagger} \hat{a}^{(\alpha)} + \frac{1}{2} \sum_{\alpha, \beta, \gamma, \zeta=0}^{\Omega} \lambda_0 \delta^{(\alpha, \beta, \gamma, \zeta)} \hat{a}^{(\alpha)\dagger} \hat{a}^{(\beta)} \hat{a}^{(\gamma)\dagger} \hat{a}^{(\zeta)\dagger}.
$$

In the above, $\epsilon^{(\alpha)}$ is the eigenvalue of the harmonic oscillator for state $|\alpha\rangle$, and $Q^{(\alpha, \beta)}$ is a matrix given by

$$
Q^{(\alpha, \beta)} = \langle \alpha | \hat{Q} | \beta \rangle = \begin{cases} \sqrt{\frac{\pi}{2}} & \alpha = \beta + 1 \\ \sqrt{\frac{\pi}{2}} & \beta = \alpha + 1 \\ 0 & \text{otherwise.} \end{cases}
$$

Evaluation of the $\delta^{(\alpha, \beta, \gamma, \zeta)}$ matrix is slightly more involved, as it is required to solve the integral

$$
\delta^{(\alpha, \beta, \gamma, \zeta)} = \langle \alpha, \beta|\delta(\hat{Q} - \hat{Q}')|\gamma, \zeta\rangle
$$

$$
= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{1}{2\pi} \left( \frac{1}{\pi} \right)^{1/4} e^{-Q^2/2} He^{(\alpha)}(Q) \frac{1}{\sqrt{2\pi}} \left( \frac{1}{\pi} \right)^{1/4} e^{-Q'^2/2} He^{(\beta)}(Q')
$$

$$
\times \delta(\hat{Q} - \hat{Q}') \frac{1}{2\pi} \left( \frac{1}{\pi} \right)^{1/4} e^{-Q'^2/2} He^{(\gamma)}(Q) \frac{1}{\sqrt{2\pi}} \left( \frac{1}{\pi} \right)^{1/4} e^{-Q'^2/2} He^{(\zeta)}(Q') dQ dQ'
$$

where $He^{(\alpha)}(Q)$ is a Hermite polynomial of order $\alpha$. However, an analytic solution is possible, and the above may be simplified using the relationship

$$
\int_{-\infty}^{+\infty} f(x') \delta(x - x') dx' = f(x),
$$

and like terms collated to obtain

$$
\delta^{(\alpha, \beta, \gamma, \zeta)} = \frac{1}{\pi \sqrt{2(2\alpha+2\beta+2\gamma+2\zeta)(\alpha!\beta!\gamma!\zeta!)}} \int_{-\infty}^{+\infty} e^{-2Q^2} He^{(\alpha)}(Q) He^{(\beta)}(Q) He^{(\gamma)}(Q) He^{(\zeta)}(Q) dQ.
$$
This will only be non-zero if the integrand is an even function, so the product of Hermite polynomials can only have even powers of $Q$

$$
\delta^{(\alpha,\beta,\gamma,\zeta)} = \frac{1}{\pi \sqrt{2^{\alpha+\beta+\gamma+\zeta} \alpha! \beta! \gamma! \zeta!}} \int_{-\infty}^{+\infty} e^{-2Q^2} \sum_{\tau=0} \ c_{2\tau} Q^{2\tau} \ dQ
$$

(43)

where $c_{2\tau}$ is a constant obtained from the product of Hermite polynomial coefficients. Using the following identity

$$
\int_{-\infty}^{+\infty} x^{2n} e^{-\frac{1}{2} a x^2} = \sqrt{\frac{2\pi}{a}} \ \frac{1}{a^n} (2n - 1)!! \quad \text{for } n > 0
$$

(44)

combined with a Gaussian integral for $\tau = 0$, Eq. 43 can be evaluated as

$$
\delta^{(\alpha,\beta,\gamma,\zeta)} = \frac{1}{\pi \sqrt{2^{\alpha+\beta+\gamma+\zeta} \alpha! \beta! \gamma! \zeta!}} \left[ \sqrt{\frac{\pi}{2}} c_0 + \sum_{\tau=1} \ c_{2\tau} \sqrt{\frac{\pi}{2} \frac{1}{4^\tau}} (2\tau - 1)!! \right].
$$

(45)

Initial Conditions for Application 2

The initial Fock state for the system includes all bosons in the ground harmonic state

$$
|n\rangle = \prod_{\alpha=0}^{\Omega} |n^{(\alpha)}\rangle = |n^{(0)}, n^{(1)}, \ldots, n^{(\Omega)}\rangle = |100, 0, \ldots, 0\rangle.
$$

(46)

As with the double well problem, the coherent states are sampled via a gamma distribution like in Eq. 33. The ground state with occupation $n^{(\alpha=0)} = 100$ is sampled with compression parameter $\sigma^{(\alpha=0)} = 1.0$, whilst the excited states with occupation $n^{(\alpha>0)} = 0$ are sampled with compression parameter $\sigma^{(\alpha>0)} = 10000$. The large compression parameter for the latter is necessary to ensure the coherent states do not become uncoupled over the course of the calculation.

Initial amplitudes are calculated by projecting the basis onto this initial Fock state

$$
\langle z_k(0)|n\rangle = \sum_{l=1}^{K} D_l(0) \langle z_k(0)|z_l(0)\rangle,
$$

(47)

where

$$
\langle z_k(0)|n\rangle = \left( \prod_{\alpha=0}^{\Omega} z_k^{(\alpha)}(0)|n\rangle \right)
$$

$$
= \langle z_k^{(\alpha=0)}(0)|n^{(\alpha=0)}\rangle
$$

$$
= e^{-\frac{|z_k^{(\alpha=0)}(0)|^2}{2}} \frac{(z_k^{(\alpha=0)*}(0))^{100}}{\sqrt{100!}}.
$$

(48)