Monte Carlo techniques for real-time quantum dynamics

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Abstract

The stochastic-gauge representation is a method of mapping the equation of motion for the quantum mechanical density operator onto a set of equivalent stochastic differential equations. One of the stochastic variables is termed the “weight”, and its magnitude is related to the importance of the stochastic trajectory. We investigate the use of Monte Carlo algorithms to improve the sampling of the weighted trajectories and thus reduce sampling error in a simulation of quantum dynamics. The method can be applied to calculations in real time, as well as imaginary time for which Monte Carlo algorithms are more-commonly used. The method is applicable when the weight is guaranteed to be real, and we demonstrate how to ensure this is the case. Examples are given for the anharmonic oscillator, where large improvements over stochastic sampling are observed.

Key words: quantum dynamics, Monte Carlo, Metropolis algorithm, branching algorithm, stochastic gauges, Bose Einstein condensation

1 Introduction

Complexity is a fundamental problem in theoretical physics [1]. It refers to the large size of many physical systems in terms of their microscopic constituents, and therefore the near impossibility to predict, from first principles, the detailed properties of such a system. In quantum physics the problem

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is manifest as the enormous dimension of the appropriate Hilbert space for most realistic physical systems. In particular, the calculation of exact quantum dynamics is notoriously difficult, because the dimension of the Hilbert space scales exponentially with the number of modes. This enormous Hilbert space prevents complete representation of the evolving many-body quantum state as a numerical state-vector for large many-body systems. Successful quantum simulation methods can thus only hope to sample the quantum evolution, to some finite precision, by use of stochastic methods.

Such quantum Monte Carlo (QMC) techniques have a long history in first-principles, microscopic calculations of thermal equilibrium and ground states in quantum systems [2,3]. Certain classes of QMC methods, such as diffusion or Green’s function approaches [4] (projector methods) are restricted to calculation of ground state properties. Methods based on path integrals [5] are a simulation through imaginary time, and can calculate correlations at any temperature. However, when it comes to real-time calculations (i.e. dynamics), path integral QMC methods become difficult because of sign or phase problems [6,7].

An alternative approach is provided by phase-space representations [8,9,10], which can be used to map quantum dynamics to a set of equivalent stochastic differential equations. The number of phase-phase equations scale polynomially with the number of modes, allowing computationally tractable simulations. Phase-space methods have proved useful in the past for simulating quantum dynamics, particularly in the field of quantum optics [11,12,13] A natural extension of these techniques is to the field of degenerate quantum gases, where the interacting particles are atoms or molecules rather than photons [14,15]. Recently it has been discovered that Fermi gases can be treated with related techniques [16,17].

The mapping of a quantum problem to phase-space equations is far from unique. This nonuniqueness can be exploited to tailor the form the stochastic equation without affecting the physical, ensemble result. The different choices correspond to different “stochastic gauges”. In this paper, we use this freedom to generate stochastic equations with real weights, which we then sample with Monte Carlo techniques. The real weights avoid the sign or phase problem encountered in other QMC approaches to quantum dynamics. Since the stochastic gauge method is a relatively new technique, we choose to focus here on an especially simple case with known exact solutions, in order to clarify the problems and advantages of this real weight approach.

We emphasise, however, that even the simple case of the quantum anharmonic oscillator that we treat here has highly nontrivial behaviour when treated as a stochastic problem. It is also relevant to current experiments on the dynamics of ultra-cold atoms trapped in optical lattices. These are described
rather accurately by the so-called Bose-Hubbard model, which reduces to the type of single-mode theory treated here in the Mott-insulator limit in which inter-well tunneling is suppressed. We simulate the decay of coherence due to phase-diffusion, a physical effect that has already been experimentally observed in recent BEC experiments [18]. The present paper focuses on this relatively straightforward and exactly soluble case, in order to demonstrate the important principles behind first-principles quantum dynamical simulation in real time. Due to the linear scaling of these methods with increasing numbers of modes, we expect that the same basic ideas will apply to multi-mode or multi-well situations where there are no known exact solutions in general.

This paper is organised as follows. In Sec. 2 we review the stochastic-gauge representation [19] and motivate the use of Monte Carlo techniques for sampling the weighted stochastic trajectories. In Sec. 3 we introduce a simple model for interacting quantum dynamics, and describe the design of a gauge that results in real weights.

In Sec. 4 we review the Metropolis-Hastings algorithm [20,21,22] and describe its application to stochastic-gauge simulations, demonstrating the improvements over the usual stochastic sampling for the same type of gauge.

In Sec. 5 we describe an alternative scheme, based on stochastic sampling, but with a branching algorithm for efficient handling of the weights.

Finally, in Sec. 6 we discuss the advantages and disadvantages of each Monte Carlo method in the context of future applications.

2 The Stochastic-Gauge Representation

The stochastic-gauge (or gauge-$P$) representation is a generalisation of the positive-$P$ ($+P$) representation [9,10], where the density operator is expanded as a positive distribution over an off-diagonal, over-complete basis set of coherent states. The essential difference between the $+P$ and the stochastic-gauge representation is that the later is defined over a quantum phase space with an additional dimension termed the weight $\Omega$, such that the total phase space vector is $\vec{\alpha} = (\alpha, \beta, \Omega)$ of complex dimension $2M + 1$. Throughout this paper the $+P$ variables $(\alpha, \beta)$ are referred to as mode variables. For a complete description of the method we refer the reader to Ref. [19], however we briefly summarise the main features of the method below.

The procedure for calculating quantum dynamics using the stochastic-gauge representation is similar to that using the $+P$ representation and involves deriving, via a Fokker-Planck equation, a set of stochastic differential equa-
tions equivalent to the original quantum master equation. The most general quantum-dynamical evolution may be written as a master equation of the form
\[ \frac{\partial \hat{\rho}}{\partial t} = L[\hat{\rho}], \tag{1} \]
were \( L \) is a Liouville superoperator (e.g. \( L[\hat{\rho}] = -i[\hat{H}, \hat{\rho}] \) for unitary evolution).

To calculate the quantum dynamics using the stochastic-gauge representation we expand the density operator in an over-complete basis set as
\[ \hat{\rho} = \int d^{4M+2} \alpha G(\alpha, \alpha^*) \Lambda(\alpha), \tag{2} \]
where
\[ \Lambda(\alpha) = \Omega ||\alpha|| \langle \beta^* \rangle \exp[-\alpha \cdot \beta], \]
\( G(\alpha, \alpha^*) \) is the (non-unique) gauge distribution function, and
\[ ||\alpha|| = \sum_n \frac{\alpha_n}{\sqrt{n!}} |n\rangle \tag{3} \]
is a Bargmann coherent state [10].

By use of operator identities for creation and annihilation operators acting on the kernel and subsequent integration by parts (with the assumption that boundary terms vanish), it is possible to show that any master equation involving only two-body terms is equivalent to a gauge distribution function evolving according to a positive-definite Fokker-Planck equation. The dynamical moments may therefore be obtained by evolving an equivalent set of stochastic differential equations (SDEs) and taking stochastic averages of an appropriate product of stochastic variables [23].

At this stage it is possible to add arbitrary terms to the Fokker-Planck differential operator that give zero when acting on the kernel. These terms cannot affect the quantum averages, but add stochastic gauges — arbitrary functions on phase space — to the drift part of the corresponding SDEs [19]. The central result is easy to state. For an \( M \) mode quantum system with \(+P\) Ito equations of the form
\[ \dot{\alpha} = \bar{A}(\alpha) + \bar{B}^{(+)} \xi, \tag{4} \]
where \( \bar{A}(\alpha) \) and \( \bar{B}^{(+)} \) are the positive-\( P \) drift vector and diffusion matrix, respectively, then the stochastic-gauge equations for the system are
\[ \dot{\alpha} = \bar{A}(\alpha) + \bar{B}^{(+)} \left( \xi - \bar{g} \right), \tag{5} \]
\[ \dot{\Omega} = \Omega \bar{g}^T \xi. \tag{6} \]

Here \( \bar{g} = \bar{g}(\alpha) \) is a vector of \textit{stochastic gauges} and \( \bar{\xi} \) is a vector of gaussian noises where
\[ \left\langle \xi_i(t) \xi_j(t') \right\rangle = \delta_{ij} \delta(t - t'). \tag{7} \]
The stochastic gauges $\vec{g}$ can be used to modify the deterministic evolution of the stochastic trajectories and are therefore called drift gauges.

Also possible are diffusion gauges which arise from the non-unique factorisation of drift matrix $D$ appearing in the Fokker-Planck equation into a noise matrix $B$ for the SDEs, where

$$D = BB^T.$$  \hspace{1cm} (8)

Diffusion gauges can be used, for example, to “squeeze” the noise between stochastic variables to improve sampling [24]. More general types of diffusion gauge are possible in the full stochastic-gauge formalism [19,25].

For a single mode, quantum-dynamical averages of normally ordered products of creation and annihilation operators are calculated as stochastic averages in the following manner

$$\langle (\hat{a}^\dagger)^m \hat{a}^n \rangle_{QM} = \frac{\langle \Omega \beta^m \alpha^n + (\Omega \beta^n \alpha^m)^* \rangle_{stoch}}{\langle \Omega + \Omega^* \rangle_{stoch}}.$$  \hspace{1cm} (9)

In principle any gauge that does not introduce boundary terms on partial integration will reproduce the exact quantum averages in the limit that an infinite number of trajectories are simulated, and so all gauges represent the same physics. However, in practice we may only simulate a finite number of trajectories due to limited computing resources, and so we would like to choose a gauge that gives rise to the most compact phase space distribution $G(\vec{a}, \vec{a}^*, t)$ possible. A narrower distribution means that fewer stochastic trajectories need to be sampled to obtain quantum averages with a given accuracy. The situation is similar to classical or quantum electrodynamics, where a judicious choice of gauge simplifies the solution of certain problems.

### 2.1 Monte Carlo techniques for the weight variable

The motivation for this work is that in the stochastic gauge representation, stochastic trajectories are often generated with weights that vary over many orders of magnitude as illustrated in Fig. 1. From Eq. (9) we can see that the trajectories with relatively high weight contribute more to the overall stochastic averages than those with relatively low weight.

The situation is analogous to path-integral calculations of quantum averages in imaginary time (thermal quantum averages), where quantum Monte Carlo techniques have long been used to sample the weight parameter more efficiently [26,4]. In the standard stochastic gauge prescription the stochastic trajectories are generated randomly. If the weight parameter can be interpreted
as a probability, then this suggests that more sophisticated Monte Carlo techniques can be used to efficiently sample high-weight trajectories, thus improving the sampling of physical averages. In this paper we focus on real-time dynamics, although the same techniques apply to imaginary-time stochastic gauge calculations [17]. Previously Monte Carlo techniques have had limited success with real-time quantum dynamics, where path-integral approaches are plagued by sign problems due to the rapidly-oscillating phase [3,27].

However, there is a complication — in the stochastic-gauge representation the weight is complex in general. In principle it is possible to apply Monte Carlo techniques to problems with a complex weight — by treating the modulus of the weight as the ‘importance’. In practice, however, sign problems are encountered when the phase of the weight eventually becomes evenly distributed around the unit circle in the complex plane. In order to strictly interpret the weight as a probability distribution, we must ensure that our choice of gauge leads to a weight parameter that is real. This means that the gauge functions we introduce must also be real.

3 Example: The Kerr Anharmonic Oscillator

In this section we introduce a single-mode boson model for quantum nonlinear dynamics — the Kerr anharmonic oscillator. The Hamiltonian is

\[ \hat{H} = \hbar \omega_0 (\hat{a}^{\dagger} \hat{a} + \frac{1}{2}) + \frac{1}{2} \kappa \hat{a}^{\dagger 2} \hat{a}^2 = \hbar \omega_0 (\hat{n} + \frac{1}{2}) + \frac{1}{2} \kappa \hat{n} (\hat{n} - 1), \tag{10} \]

where \( \hat{n} = \hat{a}^{\dagger} \hat{a} \) is the number operator. Traditionally this Hamiltonian has been used to describe the Kerr effect in nonlinear optics. It has received renewed interest recently, as it is the restriction to a single site of the Bose-Hubbard model. This has been shown to describe ultra-cold bosonic atoms in an optical lattice [28], a topic of recent theoretical and experimental interest [29,30].

Throughout this paper we work in the interaction picture with

\[ H_{\text{int}} = \frac{1}{2} \kappa \hat{a}^{\dagger 2} \hat{a}^2. \tag{11} \]

A number state is an eigenstate of this Hamiltonian. Introducing the dimensionless time \( \tau = \kappa t / \hbar \), a number state evolves according to

\[ |n(\tau)\rangle = \exp(-in(n - 1)\tau/2)|n(0)\rangle \tag{12} \]

Hence, any initial state can be decomposed into number states and an exact solution found. In particular, for an initial coherent state \( |\psi(0)\rangle = |\alpha\rangle \) with \( \alpha \)
Fig. 1. Illustration of the spreading of weights in a stochastic gauge simulation for the anharmonic oscillator. These three trajectories of $\Omega$ were generated using randomly chosen noises for a real-gauge simulation of the anharmonic oscillator ($A = 2, \lambda = 1/2$), as described in Sec. 3.1, with mean atom number $\bar{n} = 100$. The total simulation time was $\tau_{\text{tot}} = 1/\sqrt{\bar{n}} = 0.1$ and the time step used was $\Delta \tau = \tau_{\text{tot}}/10^3 = 10^{-4}$. Note that the relative weights of the trajectories vary in time so the Metropolis algorithm can only be targeted to sample the distribution at a single chosen time. The branching algorithm clones and kills trajectories continuously in time in proportion to their weight so as to obtain continuous-time samples of the distribution.

real, the solution is

$$|\psi(\tau)\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} \exp(-in(n-1)\tau/2)|n\rangle,$$  \hspace{1cm} (13)

As this model both has an exact solution and includes the nonlinearity that is a feature of models such as the Bose-Hubbard Hamiltonian, it forms an excellent testing ground for quantum simulation methods [31].

An important quantum feature of this Hamiltonian is that given an initial coherent state $\hat{\rho}(0) = |\alpha\rangle\langle\alpha|$ with mean boson number $\bar{n} = |\alpha|^2$, the dynamics display a series of collapses and revivals. Defining the quadrature variables

$$\hat{X} = (\hat{a} + \hat{a}^\dagger)/2, \quad \hat{Y} = (\hat{a} - \hat{a}^\dagger)/2i,$$  \hspace{1cm} (14)

we find there are three characteristic timescales for anharmonic oscillator...
dynamics. The quadratures initially undergo oscillations with period \( \tau_{\text{osc}} \sim O(1/\bar{n}) \), which are damped to zero over a time of \( \tau_{\text{coll}} \sim O(1/\sqrt{\bar{n}}) \). However, the oscillations revive at time \( \tau_{\text{rev}} \sim O(1) \), which for a large mean boson number can be many times the collapse time.

Because the period of oscillation of the quadratures can be very short for large mean atom number, and because we are most interested in the envelope of the collapse, we choose to perform the calculations in a rotating frame. The angular frequency of the rotation is equal to the mean atom number, and the \( X \)-quadrature, whose exact solution is

\[
\langle \hat{X}(\tau) \rangle = \sqrt{\bar{n}} e^{\bar{n}(\cos(\tau) - 1)} \cos(\bar{n}(\sin(\tau) - \tau)),
\]

(15)
collapses dynamically for large mean atom number according to:

\[
\langle \hat{X}(\tau) \rangle \simeq \sqrt{\bar{n}} e^{-\bar{n}\tau^2}.
\]

(16)

For the anharmonic oscillator Hamiltonian the stochastic-gauge Stratonovich SDEs are

\[
\dot{\alpha} = -i\alpha^2 \beta + i\alpha/2 + \sqrt{-\alpha} \cosh(A)(\xi_\alpha - g_\alpha) \\
\dot{\beta} = i\beta^2 \alpha + i\beta/2 + \sqrt{i\beta} \sinh(A)(\xi_\beta - g_\beta) \\
\dot{\Omega} = \Omega \sum_{j=\alpha,\beta} g_j \xi_j.
\]

(17) \hspace{1cm} (18) \hspace{1cm} (19)

Here \( A \) is a diffusion gauge that we choose to be constant in this paper, \( g_j, j = \alpha, \beta \) are drift gauges to be chosen subsequently, and \( \xi_j \) are dimensionless Gaussian noise terms chosen so that:

\[
\langle \xi_i(\tau) \xi_j(\tau') \rangle = \delta_{ij} \delta(\tau - \tau').
\]

(20)

For better numerical performance we choose to work with \textit{log variables}:

\[
\theta = (1/2) \log(\alpha \beta), \quad \phi = (1/2i) \log(\alpha/\beta), \quad \omega = \log(\Omega).
\]

(21)

These obey the following Stratonovich SDEs:

\[
\dot{\theta} = -ie^{-A}(\xi_1 - g_1 - i(\xi_2 - g_2)),
\]

(22)

\[
\dot{\phi} = -e^{2\theta} + \frac{1}{2} - \frac{1}{2} e^A(\xi_1 - g_1 + i(\xi_2 - g_2)),
\]

(23)

\[
\dot{\omega} = S \omega + \sum_{j=1,2} g_j \xi_j,
\]

(24)
where we have defined the linearly transformed noises $\xi_1 = (\xi_\alpha + \xi_\beta)/\sqrt{2}$ and $\xi_2 = (\xi_\alpha - \xi_\beta)/\sqrt{2}$, which obey the same statistics, and similarly $g_1 = (g_\alpha + g_\beta)/\sqrt{2}$ and $g_2 = (g_\alpha - g_\beta)/\sqrt{2}$. The term $S_\omega$ is a Stratonovich correction factor which depends on the gauge choice, and will be calculated for each specific case. We note here that, unlike in the corresponding classical oscillator equations, both $\theta = \theta_X + i\theta_Y$ and $\phi = \phi_X + i\phi_Y$ are intrinsically complex.

3.1 Choice of Gauge

In this section we discuss possible choices of diffusion gauge for the anharmonic oscillator with a view to using Monte Carlo techniques to sample the weight.

In Ref. [32] Drummond and Deuar investigated the following drift-gauge choice for the anharmonic oscillator

$$g_1 = ig_2 = ie^{A+2\theta_X} \sin(2\theta_Y),$$

(25)

where the $X$ and $Y$ superscripts refer to the real and imaginary parts of the phase-space variable respectively (this notation is used throughout this paper). They found that this gauge extended simulation times by many orders of magnitude for the same number of stochastic trajectories. In particular they could simulate well past the collapse time for an initial coherent state.

As noted in Sec. 2.1, for the Monte Carlo methods to be successful it is highly desirable to have a real weight. Unfortunately the above choice of gauge is complex and thus leads to complex weights. We have trialled the use of Monte Carlo techniques based on using the modulus of the weight, but found these to be unsuccessful due to the phase problem described in the introduction.

In order to have real weights, we would like to design a real gauge with similar properties to the above complex gauge to give a similar extension of simulation time. The reason that the complex gauge Eq. (25) improves simulation times is that it removes a driving term from the imaginary part of the $+P \phi$ equation. The presence of this term forces trajectories to diverge to infinity in a non-classical direction in phase-space ($\phi_Y \to \pm \infty$), thus resulting in large sampling errors. At the same time the equations for $\theta$ and the real part of $\phi$ are unaffected due to a cancellation between $g_1$ and $g_2$. We could remove the offending term from the $\phi_Y$ equation with a single real gauge $g_2$, however this would necessarily appear in the $\theta_Y$ equation leading to an instability that causes poor sampling.

Thus it seems that a drawback to choosing real gauges is that there is substantially less control over the stochastic trajectories. This could have been anticipated because, in general, with a complex gauge we have as many gauge
degrees of freedom as we do real phase space dimensions, $4M$ (excluding the weight dimensions). However with real gauges we only have half as many gauge degrees of freedom, $2M$, meaning that we cannot independently control the drift in the real and imaginary components of each of the mode variables.

An additional source of gauge freedom is obtained from choosing a non-square noise matrix in deriving the SDEs. This freedom was pointed out in [19] but not explored. Specifically, it is possible to take the noise matrix to be of the general form

$$
B = [B_0, Q],
$$

where $B_0$ is a square ($2M \times 2M$) noise matrix such that $B_0B_0^T = D - QQ^T$, and $Q$ is a $2M \times W$ matrix whose entries are arbitrary complex functions. This choice reproduces the correct moments in the limit of a large number of stochastic trajectories, but introduces more than the minimum number of noise terms into the stochastic equations. Naively this could be expected to lead to worse sampling errors. However, this additional gauge freedom allows us to overcome the restrictions of the standard real gauges and improve the sampling overall.

For the anharmonic oscillator we choose

$$
Q = \begin{bmatrix} 0 & 0 \\ \lambda & i\lambda \end{bmatrix},
$$

in the $(\theta, \phi)$ variables, where $\lambda$ could be an arbitrary complex function on phase space, although we choose it to be constant in our example. Here $Q$ satisfies $QQ^T = 0$ so the other noise terms are unaffected. In doing so we have added a term of the form $\lambda(\xi_3 + i\xi_4)$ to the equation of motion for $\phi$, Eq. (23). An equivalent way of understanding this additional noise is that due to the analytic nature of the stochastic gauge kernel we have

$$
\lambda \left( \frac{\partial^2}{\partial \phi_X^2} + \frac{\partial^2}{\partial \phi_Y^2} \right) \Lambda(\vec{\alpha}) = 0.
$$

Thus we are free to add $\lambda(\partial^2/\partial \phi_X^2 + \partial^2/\partial \phi_Y^2)$ to the Fokker-Planck differential operator without affecting the physical moments.

We are now able to introduce additional gauges to the $\dot{\phi}$ equation in the manner described in [19] so that the extra term in the $\dot{\phi}$ equation becomes

$$
\lambda((\xi_3 - g_3) + i(\xi_4 - g_4)),
$$

and the gauges $g_3$ and $g_4$ enter the weight equation in the same way as the other drift gauges. The extra noise allows us to control the $\phi_Y$ divergence using only a real gauge, without affecting the $\theta_Y$ equation. Specifically we choose
The final SDEs that we focus on sampling for the rest of this paper are summarised as

\begin{align}
\dot{\theta} &= \frac{1}{2} e^{-A}(\xi_1 - i \xi_2), \\
\dot{\phi} &= -e^{2\theta X} \cos(2\theta Y) + \frac{1}{2} \left( e^{A}(\xi_1 + i \xi_2) - 2\lambda(\xi_3 + i \xi_4) \right), \\
\dot{\omega} &= S_\omega - \frac{e^{2\theta X}}{\lambda} \sin(2\theta Y) \xi_4,
\end{align}

where \( S_\omega = -e^{4\theta X} \sin^2(2\theta Y)/2\lambda^2 \) is the Stratonovich correction in the weight equation. Note that although we choose \( g_3 = 0 \) it is still necessary to include the noise \( \xi_3 \) for the mapping to be exact.

Of course there are other possible choices of real gauges, but we have found this combination to be well-suited to illustrating the improvements possible with Monte Carlo sampling.

In Fig. 2 we illustrate stochastic sampling of the above SDEs. We begin with an initial coherent state with mean atom number \( \bar{n} = 100 \), and simulate to a final time of \( \tau = 1/\sqrt{\bar{n}} = 0.1 \), which is of the order of the collapse time. Clearly the sampling of the solution is only accurate for short times. In particular, the sampled \( \langle \Omega \rangle_{\text{stoch}} \) decays towards zero when it should remain at one for all times in a simulation of unitary dynamics. The error in sampling the mean atom number, which should remain at 100, is due almost entirely to poor sampling of the weights, as can be seen by the almost identical decay. Even worse, the estimated error in the means is small despite the fact that they are clearly far from the analytic result. This poor sampling occurs more quickly on the scale of the collapse for larger mean atom number.

This behaviour can be understood by considering the nature of the distribution of weights. We find that the weight parameter evolves with time towards zero for most trajectories. However, we know that the mean weight must be one, and so there must exist a small number of trajectories with large weights. Thus the distribution of weights seems to be skewed towards zero with a long tail extending to large weights. Such a distribution is difficult to sample, so it is not surprising that we underestimate the errors in the means as these assume Gaussian statistics. Fortunately, Monte Carlo techniques are particularly successful in sampling skewed distributions. Below we describe the
Fig. 2. Real-gauge simulation of anharmonic oscillator dynamics for an initial coherent state with mean atom number $\bar{n} = 100$ ($A = 2$, $\lambda = 1/2$). (a) Mean weight, (b) mean atom number (corresponding stochastic variable $n = \alpha \beta$) and (c) mean $X$–quadrature (corresponding stochastic variable $X = (\alpha + \beta)/2$). Averages were carried out over $10^6$ stochastic trajectories. The total simulation time was $\tau_{\text{tot}} = 1/\sqrt{\bar{n}} = 0.1$ and the time step used was $\Delta \tau = \tau_{\text{tot}}/10^3 = 10^{-4}$. The shaded region indicates the estimated error in the simulation and the stochastic means are in the centre of the region. The analytic results are shown as dashed lines. The sampling is poor except for short times due to the skewed weight distribution.
application of the Metropolis-Hastings algorithm and a Monte Carlo branching algorithm to our SDEs for the anharmonic oscillator.

4 The Metropolis-Hastings Algorithm

The Metropolis-Hastings algorithm is a well-known technique for generating samples of a multi-dimensional probability distribution. Here we briefly describe the algorithm and discuss how to estimate errors in quantities derived from such samples. In particular this may be useful for readers from the ultra-cold matter community who may be unfamiliar with these methods.

4.1 Algorithm

The Metropolis algorithm was first described in 1953 [20] and was used to sample a thermal Boltzmann distribution, which can be viewed as a probability distribution over the space of all thermally accessible states of a system. Subsequently the Metropolis algorithm has been generalised to many types of probability distributions/densities over both discrete and continuous spaces, and there is a vast amount of mathematical literature on Markov Chain Monte Carlo (MCMC) techniques (see e.g. [6,7].)

In this section we summarise the Metropolis algorithm in a more general form due to Hastings [21]. A well-written introduction to the Metropolis-Hastings algorithm may be found in [22], and here we follow their notation. Formally, the Metropolis algorithm is a MCMC technique for efficiently sampling a probability distribution, \( \pi(s) \), where \( s \in S \) represents the state of some system, and \( S \) is the domain of the distribution known as the state space. To be a true probability distribution \( \pi(\cdot) \) must be normalised \( \int ds \pi(s) = 1 \), however one of the virtues of the algorithm is that the functional form of the distribution need only be known up to a constant factor in order to apply the algorithm\(^1\).

A Markov chain can be thought of as a random walk through state space where the probability of making a particular step depends only on the current location. It is a sequence of points, \( s_1, s_2, \ldots, s_n \in S \), where the \( s_i \) are random variables such that

\[
p(s_i | s_1, s_2 \ldots s_{i-1}) = p(s_i | s_{i-1}).
\]

\(^1\) e.g. the partition function \( Z = \sum_{s \in S} e^{-E(s)/k_B T} \), where \( E(s) \) is the energy of the system in state \( s \), need not be known in order to sample the Boltzmann distribution, where the probability that the system is in state \( s \) is given by \( P(s) = e^{-E(s)/k_B T}/Z \).
The conditional density \( p(s_i|s_{i-1}) \) is known as the \textit{transition density} of the Markov chain. If there exists an \textit{invariant density} \( \pi^*(s) \) that satisfies the condition of \textit{detailed balance}

\[
\pi^*(s) = \int ds' \pi^*(s') p(s'|s), \tag{36}
\]

then it may be shown that the Markov chain converges to the distribution \( \pi(\cdot) \). More precisely, the elements of the chain \( \{s_i| i = b+1, \ldots, n\} \) are unbiased samples from the distribution \( \pi^*(\cdot) \) to within some given precision, where \( b \geq 0 \) is known as the \textit{burn-in} and represents the number of steps required for the chain to converge to within that precision.

The Metropolis-Hastings algorithm solves the problem of determining what transition density to use so as to generate a given invariant distribution. It is concerned with generating samples from some \textit{target density} \( \pi(\cdot) \), known apart from a constant factor, and does so by determining a suitable transition density for a Markov chain to converge to this distribution. To do this we require a \textit{candidate generating density}, \( q(s, s') \), where \( \int q(s, s') ds' = 1 \), which selects the next point in the Markov chain. The \textit{acceptance probability} of this step is

\[
\alpha(s, s') = \min \left( \frac{\pi^*(s') q(s', s)}{\pi^*(s) q(s, s')}, 1 \right). \tag{38}
\]

The Metropolis-Hastings algorithm can be summarised as follows

1. \textit{repeat for} \( i = 1, 2, \ldots, n \)
2. \textit{generate} \( s' \) from \( q(s_i, \cdot) \) and a uniform random variable \( u \) between 0 and 1.
3. \textit{if} \( u \leq \alpha(s_i, s') \) \textit{then set} \( s_{i+1} = s' \); \textit{else set} \( s_{i+1} = s_i \).
4. \textit{return} \( \{s_i| i = 1, 2, \ldots, n\} \)

The Metropolis-Hastings algorithm generates a Markov chain in the state space with a transition density \( p_{mh}(s'|s) = q(s, s') \alpha(s, s') \). When a proposed move is rejected the chain remains where it is. This choice of transition density ensures that the condition of detailed balance is satisfied and hence the Markov chain converges to the required target density. The algorithm generates a Markov chain that finds regions in state space where the probability distribution is peaked and samples these region with the correct frequency.

The efficiency of the algorithm is dependent on the choice of candidate generating function. Indeed the optimal choice of \( q(s, s') \) for a particular target density remains an active area of research today. An important special case
occurs if the candidate generating distribution is symmetric, $q(s, s') = q(s', s)$, and so
\[ \alpha(s, s') = \min \left( \frac{\pi(s')}{\pi(s)}, 1 \right). \]
This was Metropolis’s original formulation which was generalised to the case of an asymmetric candidate generating function in 1970 by Hastings [21].

4.2 Estimating sampling error

In general we wish to determine the weighted average over all possible states of some observable of the system
\[ \langle O \rangle_\pi = \int ds \pi(s) O(s). \]
Because the Metropolis algorithm produces a set samples of the distribution $\pi(\cdot)$, \{s_i | i = b + 1 \ldots b + n\}, such averages can be estimated as
\[ \langle O \rangle_\pi \simeq \frac{\sum_{i=b+1}^{b+n} O(s_i)}{n}. \]
The statistical uncertainty in such a quantity can be difficult to estimate because the samples are generally correlated with one another, as the samples produced by the Metropolis algorithm are not independent. One way to obtain less correlated samples is to only take every $g^{th}$ point in the chain after the burn-in for the purpose of calculating averages, where $g$ is known is the gap. However, this does not usually produce more accurate estimates of averages than could have been obtained by simply taking every sample after the burn-in.

Alternatively, one can accept the fact that the samples are correlated, but attempt to account for the correlations in some quantitative way. A scheme for estimating errors in means calculated from correlated Monte Carlo data may be found in [33].

For large dimensional state spaces one may still not be satisfied with estimating errors from a single Markov chain, even if the correlations are accounted for. An example is the sampling of probability density with multiple peaks, which may not individually give correct averages for state-space dependent quantities. In this case, the simplest procedure is to run multiple Markov chains of the same type but with different starting points, and treat the averages obtained from each chain as samples of the mean of the quantity of interest. The overall mean is calculated by
\[ \langle O \rangle = \frac{\sum_{i=1}^{\tilde{N}} \langle O \rangle_i}{N}, \]
where \( \langle O \rangle_i, i = 1 \ldots \tilde{N} \) are the means from the independent Markov chains as in Eq. (40), and the subscript \( \pi \) has been omitted for clarity. By the central limit theorem one would expect samples obtained in this way to approach a Gaussian distribution about the true mean. Therefore an estimate of the error in the mean, for \( \tilde{N} \) independent Markov chains is

\[
\Delta \left[ \langle O \rangle \right] = \sqrt{\frac{\sum_{i=1}^{\tilde{N}} \left( \langle O \rangle_i - \langle O \rangle \right)^2}{\tilde{N} - 1}},
\]

where \( \Delta[\cdot] \) denotes the error in the mean of the quantity of interest. This notation for error in the mean is used throughout this paper when referring to means obtained from Metropolis data.

4.3 Metropolis-Hastings Algorithm for the Stochastic Gauge Formalism

The appearance of the weight \( \Omega \) as a multiplicative factor in the stochastic averages in Eq. (9) suggests an interpretation as a probability distribution. In this section we show that it is possible to interpret the weight as a probability distribution over the space of all noise, and hence apply the Metropolis-Hastings algorithm.

For the purposes of computer simulation, time is necessarily discretised. To simulate the time evolution of a system for a period \( T \) we divide the time domain into \( N + 1 \) points so that each step forward in time is of length \( \Delta \tau = T/N \). For an \( M \) mode system with the standard set of drift gauges (i.e. without the extra gauges and noises discussed in Sec. 3.1) we require \( 2M \) Gaussian distributed random numbers for each step forward in time, and thus \( 2MN \) random numbers to evolve an entire trajectory. Hence our fundamental object is a \( 2MN \)-component vector of Gaussian distributed random numbers \( \vec{w} \in \mathbb{R}^{2MN} \), called the noise vector. The different realisations of \( \vec{w} \) give rise to different stochastic trajectories. The values of all stochastic phase space variables after \( N \) time steps are thus functions of \( \vec{w} \)

\[
\vec{\alpha} = \vec{\alpha}[\vec{w}], \quad \Omega = \Omega[\vec{w}].
\]

The stochastic average of some some quantity, \( \langle O \rangle_{\text{stoch}} \) is

\[
\langle O \rangle_{\text{stoch}} = \int d^{2MN} \vec{w} P(\vec{w}) O(\vec{w}) = \lim_{n \to \infty} \frac{\sum_{i=1}^{n} O[\vec{w}_i]}{n},
\]

where the \( \vec{w}_i \) are drawn from a multi-dimensional Gaussian normal distribu-
\[ P(\vec{w}) = \frac{1}{(2\pi)^{MN}} \exp \left( -\frac{\vec{w}^2}{2} \right), \]  
\[ \text{and } O = O[\vec{w}] \text{ is some quantity depending on the noise.} \]

Hence the stochastic sampling of moments in stochastic gauge simulations, Eq. (9), is the sampling of a multi-dimensional integral
\[ \langle \Omega(\vec{w})O_{mn}(\vec{w}) \rangle_{\text{stoch.}} = \int d^{2MN} \vec{w} P(\vec{w}) \Omega(\vec{w}) O_{mn}(\vec{w}), \]
where \( O_{mn}(\vec{w}) = \beta[\vec{w}]^m \alpha[\vec{w}]^n + (\beta[\vec{w}]^n \alpha[\vec{w}]^m)^* \).

The Metropolis-Hastings algorithm can be applied by identifying the state space \( S = \mathbb{R}^{2MN} \) and the state \( s \) as the vector of noises \( \vec{w} \). The probability distribution we wish to sample is
\[ \pi(\vec{w}) = \frac{P(\vec{w}) \Omega[\vec{w}]}{\mathcal{N}}, \]
where \( \mathcal{N} = \int d^{2MN} \vec{w} P(\vec{w}) \Omega[\vec{w}] \) is a normalisation constant. The Metropolis algorithm can be used to generate a set of samples of \( \pi(\vec{w}) \), \( \{\vec{w}_i| i = 1 \ldots n\} \) and estimate quantum averages as
\[ \langle (\hat{a}^\dagger)^m \hat{a}^n \rangle_{\text{QM}} = \frac{\mathcal{N}\langle O_{mn}\rangle_{\pi}}{2\mathcal{N}} = \frac{\langle O_{mn}\rangle_{\pi}}{2} \approx \frac{\sum_{i=1}^n O_{mn}[\vec{w}_i]/n}{2}. \]

None of these steps require explicit knowledge of the normalisation constant \( \mathcal{N} \), although in real-time unitary calculations we know analytically that it should always be one. Typically we run multiple Markov chains as described in Sec. 4 to obtain means and standard-deviation error estimates, \( \langle O_{mn}\rangle_{\pi} = \langle O_{mn}\rangle / \sum_{i=1}^N O_{mn}[\vec{w}_i] \).

For comparison, ordinary stochastic sampling uses a Gaussian normal random number generator to generate samples, \( \{\vec{w}_i| i = 1 \ldots N\} \), of \( P(\vec{w}) \) and calculates quantum averages as
\[ \langle (\hat{a}^\dagger)^m \hat{a}^n \rangle_{\text{QM}} \approx \frac{\sum_{i=1}^n \Omega[\vec{w}_i] O_{mn}[\vec{w}_i]/n}{2}. \]

Finally we note that the Metropolis-Hastings algorithm as outlined above only optimises the stochastic sampling of moments at the final target time. At earlier times the probability distribution \( \tilde{\pi}(\vec{w}) \) (where \( \vec{w} \) is the noise vector \( \vec{w} \) truncated at the point corresponding to the earlier time) is different in that
\[ \text{2 Other noise distributions are possible as the central limit theorem ensures Gaussian statistics in the limit of infinitesimal step size — however we use Gaussian statistics here.} \]
\( \bar{\pi}(\tilde{w}^\prime)/\bar{\pi}(\tilde{w}) \neq \pi(w^\prime)/\pi(w), \) and so we should not expect the Metropolis algorithm targeted to the later time to correctly sample the moments at earlier times. This is also illustrated in Fig. 1 where the relative weights vary considerably as time progresses.

### 4.4 Designing a Candidate Generating Function

The choice of candidate generating function \( q(\bar{w}, \bar{w}^\prime) \) is a subtle problem and perhaps the most crucial element of applying the Metropolis-Hastings algorithm to the stochastic gauge formalism. The Metropolis algorithm generates a Markov chain in noise space, where at each step the candidate generating function proposes a new noise \( \tilde{w}^\prime \) for the stochastic trajectory which is then accepted or rejected based on the acceptance probability defined by Eq. (38)

\[
\alpha(\bar{w}, \bar{w}^\prime) = \min \left( 1, \frac{\pi(\tilde{w}^\prime)q(\tilde{w}^\prime, \tilde{w})}{\pi(\tilde{w})q(\tilde{w}, \tilde{w}^\prime)} \right) = \min \left( 1, \frac{P(\tilde{w}^\prime)\Omega(\tilde{w}^\prime)q(\tilde{w}^\prime, \tilde{w})}{P(\tilde{w})\Omega(\tilde{w})q(\tilde{w}, \tilde{w}^\prime)} \right).
\]

The evaluation of the weight at the target time for the proposed noise \( \Omega(\tilde{w}^\prime) \) is a non-local procedure; even if only a single noise is altered in the time domain the entire trajectory from that time on has to be evolved until the target time in order to evaluate the new weight.

To separate the issue of sampling high weight trajectories from the Gaussian nature of the noise it is advisable to choose a candidate generating function such that

\[
\frac{q(\bar{w}, \bar{w}^\prime)}{q(\bar{w}, \bar{w}^\prime)} = \frac{P(\bar{w})}{P(\bar{w}^\prime)}. \tag{47}
\]

For this class of generating functions, the probability of a move being accepted is

\[
\alpha(\bar{w}, \bar{w}^\prime) = \frac{\pi(\tilde{w}^\prime)q(\tilde{w}, \tilde{w}^\prime)}{\pi(\tilde{w})q(\tilde{w}, \tilde{w}^\prime)} = \frac{\Omega(\tilde{w}^\prime)P(\tilde{w}^\prime)q(\tilde{w}, \tilde{w}^\prime)}{\Omega(\tilde{w})P(\tilde{w})q(\tilde{w}, \tilde{w}^\prime)} = \frac{\Omega(\tilde{w}^\prime)}{\Omega(\tilde{w})}, \tag{48}
\]

which is only dependent on the weight rather than the Gaussian distribution, \( P(\cdot) \).

### 4.5 Time and frequency domain noise functions

A simple generating function of this type is selecting a number of entries in the current noise vector and generating new noises for these. This procedure can be carried out in either the time or the frequency domain of the noise. If the noises are altered in the time domain the stochastic trajectory is clearly unaltered up until the point of the first change. If noises are altered in the frequency domain then every noise in the time domain is affected to some
extent. We consider altering noises in the frequency domain to be a more natural “small-step” for the Metropolis algorithm as all time-domain noises are changed by a small amount on average. All results presented in this paper use a generating function operating in the frequency domain.

In more detail, consider the $R$ independent noise vectors of length $N$, $\vec{w}_j \in \mathbb{R}^N$, $j = 1 \ldots R$, separately, instead of a single noise vector of length $RN$. Insight into strategies for altering noises may be gained by taking the discrete Fourier transform of each noise vector

$$\vec{K}_j(n) = \sum_{k=0}^{N-1} e^{2\pi i kn/N} \vec{w}_j(k).$$

Here a subscript is used to denote each of the $R$ noise vectors, and should not be confused with the notation $\vec{w}_i$ used previously to denote the sequence of noise vectors in a Markov chain. Brackets $(\cdot)$ denote the components of the noise/spectrum vectors. The $n = 0$ component of $\vec{K}$ is the mean of the noise, and the fact that the noise is real places constraints on the components. Let $\mathcal{N}(\mu, \sigma)$ denote a Gaussian distribution of mean $\mu$ and standard deviation $\sigma$. The Fourier transform of a vector whose components are normally distributed real variables ($\vec{w}(n)$ distributed as $\mathcal{N}(0, 1)$) is complex. For even $N$ the real and imaginary parts of each component in the range $2 \leq n \leq N-1$ are distributed as $\mathcal{N}(0, \sqrt{N}/2)$ and subject to the constraint $\vec{K}(N-n) = \vec{K}(n)^*$, while the $n = 1$ and $n = N$ components are real and distributed as $\mathcal{N}(0, \sqrt{N})$. For odd $N$, the real and imaginary parts of each component in the range $2 \leq n \leq N$ are distributed as $\mathcal{N}(0, \sqrt{N}/2)$ and subject to the constraint $\vec{K}(N-n) = \vec{K}(n)^*$, while only the $n = 1$ component is real and distributed as $\mathcal{N}(0, \sqrt{N})$. These constraints preserve the total number of independent components $N$.

It is informative to study an individual trajectory and alter noise elements individually in frequency space to gauge the effect on the final weight. One might expect that the low frequency noise should be more important than the high frequency noise, as high frequency noise should “average out” over a shorter time scale and thus not affect the dynamics as much. We find that this is true and Fig. 3 quantifies the potential of frequency components of the noise to affect the final value of the weight. To obtain this graph four random noise vectors were generated and the corresponding stochastic trajectory evolved using real gauge discussed in Sec. 3.1 with mean atom number, $\bar{n} = 100$, and diffusion gauge $A = 2$. Using this initial trajectory as a starting point, a particular component of the noise spectrum was examined for its effect on the final weight by choosing $10^3$ random values for that component and evolving the corresponding stochastic trajectory, with all other components of the noise spectrum the same. In Fig. 3 the standard deviation of the final weights obtained in this manner is plotted on a log scale against the spectrum component number that was altered. It is clear from this figure that the low
frequency noises have greater potential to affect the final weight. This trend is independent of the initial trajectory, however we note the actual values of the standard deviations obtained vary considerably depending on the initial trajectory.

Another question to consider is how many sites in the frequency domain to alter in proposing a new noise vector, and how to select these. As the low-frequency noise seems to affect the final value of the weight more than the high-frequency noise, one might be tempted to consider strategies where low-frequency noise is altered more often so as to more effectively explore the noise space. In practice we found that such strategies were no more effective than selecting sites randomly. Typically we chose to alter of the order $1 - 10\%$ of the total components of the noise. A good guiding principle is that Metropolis sampling is thought to be most efficient when approximately 50\% of proposed moves are accepted during sampling [6,7]. We therefore experimented with different percentages with this principle in mind.

4.6 Results

We now present the results of a Metropolis sampling of the real-time dynamics of the anharmonic oscillator using the real gauge discussed in Sec. 3.1 and the candidate generating functions discussed in Sec. 4.4. To allow for the distribution $\pi(\vec{w}) = P(\vec{w})\Omega(\vec{w})/N$ to be multiply-peaked we use the more robust technique of estimating means and errors using multiple Markov chains as discussed in Sec. 4.

Figure 4 shows the Metropolis sampling of $\langle \hat{n} \rangle = \langle \hat{a}^\dagger \hat{a} \rangle$ and $\langle \hat{X} \rangle = \langle (\hat{a} + \hat{a}^\dagger)/2 \rangle$ for a real-gauge simulation of the anharmonic oscillator with $\bar{n} = 100$. We targeted the Metropolis sampling to 20 time points in intervals of $\Delta \tau = 0.005$ from 0 to the final time of $\tau = T = 1/\sqrt{\bar{n}} = 0.1$. The average at each time point is completely independent of the other time points. Altogether $n = 10^6$ samples were used for the average at each point so statistically the sampling is comparable to the stochastic sampling in Fig. 2. However because the Metropolis sampling has to be run independently for each time point and each Markov chain has to burn in before sampling begins, there is clearly a much greater computational effort required to obtain the Metropolis results. Nevertheless the Metropolis results are far more reliable than the stochastic results — at most time points the average $\langle \hat{X} \rangle$ is correct to within the estimated error. In contrast, the stochastic sampling exhibited systematic errors that were not accounted for by appropriately-large error bars.

We note that even with the Metropolis algorithm the sampled mean atom number appears to decay slightly at longer times. Although the results are still ac-
Fig. 3. Illustration of the effect of varying frequency components of the noise vectors on the final value of the weight. An initial stochastic trajectory from a real-gauge simulation of the anharmonic oscillator with mean atom number $\bar{n} = 100$ was taken as a starting point. The value of the weight at the end of the trajectory, $T = 0.5/\sqrt{\bar{n}} = 0.05$, was $\Omega = 0.9936$. The time step was $\Delta \tau = 10^{-4}$ so each noise vector contained 500 components. In frequency space each noise vector contains 250 complex components. A new random noise was chosen for a particular component of the noise vector, the entire trajectory re-evolved and the new final weight recorded. This procedure was repeated $10^4$ times for each frequency component and the variance in the final weight, $\sigma(\Omega)$, calculated. This variance is plotted versus frequency component to give a measure of the potential of each frequency component to affect the final weight. Clearly low-frequency noise has more effect than high-frequency noise.

The estimated error bars do not account for the difference from the analytic result. This behaviour, which is seen for the branching algorithm is well, is due to the inherent difficulty in sampling the skewed weight distribution even with Monte Carlo algorithms. The results are nonetheless vastly improved compared to stochastic sampling.

We experimented with different distributions of the $10^6$ allowed samples between different numbers of Markov chains. There is a trade-off between number of Markov chains and the length of the chain — if longer chains are run (e.g. $10^2$ chains each with $10^4$ samples) then the means obtained from each chain are more accurate, and closer to Gaussian about the true mean. However, there are less chains to average over compared with a run of a larger number
Fig. 4. Metropolis sampling of real-gauge simulation of anharmonic oscillator dynamics for an initial coherent state with mean atom number $\bar{n} = 100$ ($A = 2$, $\lambda = 1/2$). (a) Mean atom number, (b) mean $X$–quadrature. Metropolis averages and error estimates (crosses with error bars) were calculated from the means of $10^2$ Markov chains, each taking $10^4$ samples after a burnin of $10^4$ proposals. The total simulation time was $T = 1/\sqrt{\bar{n}} = 0.1$ and the time step used was $\Delta\tau = T/10^3 = 10^{-4}$. Proposals were generated by uniformly selecting 10% of the components of the noise vectors in the frequency domain and generating new random noise for those sites. The analytic results are shown as dotted green lines.

of shorter chains (e.g. $10^3$ chains each with $10^3$ samples). It was a matter of empirical observation to determine the best balance.

We also experimented with the fraction of noises to be altered in the frequency domain when proposing a new noise vector. As a rough guide we aimed to have 50% of proposed moves accepted during sampling. However at short times we found that even if a very large fraction of the noises were altered (e.g. 50% or more) a large fraction of proposed changes were accepted ($\sim 90\%$). This large acceptance rate is due to the distribution of weights being relatively narrow at short times. At longer times the distribution has spread out sufficiently such that lower acceptance rates are possible.

Clearly there are many parameters to be optimised in Metropolis sampling of stochastic gauge equations and we have only scratched the surface. We have aimed to present conceptually-simple approaches to illustrate the principle rather than exhaustively optimise all parameters. The fact that enormous improvements were seen over stochastic sampling — even with our very simple Metropolis schemes — gives us confidence that further improvements are possible.
5 Branching Algorithm

The second Monte Carlo technique that we investigate for real-time stochastic-gauge simulations is a branching algorithm similar to that used in Green’s function Monte Carlo, see e.g. [34]. Corney and Drummond [17] have previously used this algorithm for stochastic simulations in imaginary time using a Gaussian basis (a generalisation of the stochastic-gauge basis).

The branching algorithm is simpler to describe and more straightforward to apply to stochastic gauge simulations. Another advantage is that there are fewer free parameters than the Metropolis algorithm. The branching algorithm works by concurrently evolving a “population” of stochastic trajectories in time, and periodically cloning those that acquire a large weight and killing those that acquire a small weight.

5.1 Algorithm

We define $T$ to be the total simulation time, $\Delta \tau_b$ be the time interval between branching events and $\Delta \tau$ the fundamental time-step for integrating the SDEs. In practice it is desirable for the number of branching events $B = T/\Delta \tau_b$ and the number of time steps in a branching period $\Delta \tau_b/\Delta \tau$ to be integers. Formally the branching algorithm can be stated as

1. Begin with an initial population of $N_{\text{pop}}$ stochastic trajectories.
2. Evolve all stochastic trajectories forward in time for a period $\Delta \tau_b$
3. for $i = 1, 2, \ldots, N_{\text{pop}}$
   - Generate a uniform random variable $u$ between 0 and 1
   - Make $m_i = \text{int}[\Omega_i/\Omega + u]$ clones of trajectory $i$.
   - Set $\Omega_i = 1$
4. Set $N_{\text{pop}} = \sum_{i=1}^{N_{\text{pop}}} m_i$.

Here we set $\Omega = \langle \Omega \rangle$ to ensure that the number of trajectories in the population $N_{\text{pop}}$ remains constant on average. Because $\Omega$ does not couple into the SDEs for the mode variables, further evolution is not affected by resetting of the weights at each branching time. The statistical equivalence between the weight and the multiplicity of paths means that the physical moments are unchanged on average by the branching procedure. To see this note that the average of the mean of an observable $\bar{O}$ after the branching event is
\[
\langle O \rangle = \frac{\sum_{i=1}^{N_{\text{pop}}} \int_0^1 m_i(u) du O_i}{\sum_{i=1}^{N_{\text{pop}}} \int_0^1 m_i(u) du}
= \frac{\sum_{i=1}^{N_{\text{pop}}} \left( \Omega_i / \overline{\Omega} \right) O_i}{\sum_{i=1}^{N_{\text{pop}}} \Omega_i / \overline{\Omega}}
= \frac{1}{N_{\text{pop}}} \sum_{i=1}^{N_{\text{pop}}} \Omega_i O_i,
\]

which is identical to the mean before the branching event.

5.2 Results

In this section we present the results of a branching-algorithm sampling of real-time dynamics of the anharmonic oscillator using the real gauge discussed in Sec. 3.1. Similarly to the Metropolis sampling, we calculate averages and error estimates from multiple independent populations.

Fig. 5 shows a branching-algorithm sampling of \(\langle \hat{n} \rangle = \langle \hat{a}^\dagger \hat{a} \rangle\) and \(\langle \hat{X} \rangle = \langle (\hat{a} + \hat{a}^\dagger) / 2 \rangle\) for a real-gauge simulation of the anharmonic oscillator with \(\bar{n} = 100\). Again we see an enormous improvement in the sampling compared with stochastic sampling, Fig. 2. A clear advantage of the branching algorithm over Metropolis is that it generates physical moments at every time step as opposed to being targeted to a single time.

At each time there are, on average, \(10^6\) stochastic trajectories contributing to the stochastic averages. As with the Metropolis, it was again a matter of experimenting with different ratios of the number of trajectories to the number of populations to determine the best balance. We present results for the same division of trajectories amongst populations \((10^2\) populations of \(10^4\) trajectories\) as samples amongst Markov chains for the Metropolis algorithm so that the results are as comparable as possible.

The only free parameter in the algorithm itself is the time between branching events, \(\Delta \tau_b\). There is a trade-off between making this interval large enough that the weights spread out sufficiently for the branching to be meaningful and small enough to improve the sampling continuously in time. The branching interval used for this simulation, \(\Delta \tau_b = 10^{-3}\), is small on the scale of the dynamics of the system but large enough to allow the weights to diverge significantly between branching events.
Fig. 5. Branching-algorithm sampling of real-gauge simulation of anharmonic oscillator dynamics for an initial coherent state with mean atom number $\bar{n} = 100$ ($A = 2$, $\lambda = 1/2$). (a) Mean atom number, (b) mean $X$-quadrature. Branching averages and error estimates, indicated by the shaded region, were calculated from the means of $10^2$ populations, each containing $10^4$ trajectories on average. The total simulation time was $\tau = 1/\sqrt{\bar{n}} = 0.1$ and the time step used was $\Delta\tau = \tau/10^3 = 10^{-4}$. The branching time was $\Delta\tau_b = 10^{-3}$. The analytic results are shown as dotted lines.

6 Conclusions and Outlook

In this paper we have demonstrated the use of two Monte Carlo techniques, the Metropolis algorithm and a branching algorithm, for real-time calculations of quantum dynamics with the stochastic-gauge method. This work should be considered a proof of principle rather than a fully optimised ‘recipe’. It is part of a larger program of optimising bases, gauges and algorithms for stochastic simulations of quantum dynamics in real and imaginary time. A timely application of these methods is in theoretical calculations for ultra-cold atomic gases [35,17]. QMC methods have been used to calculate some static properties of ultra-cold gases, e.g. see [36,37]. These systems are quantum-many body by nature and hence few exact theoretical results exist. They are an ideal testing ground for theory due to their purity and well-understood controllable interactions.

In this work we have restricted ourselves to real gauges so that the weights remain real and can be interpreted as probabilities, and have considered the single-mode anharmonic oscillator as an example of our methods. In order to control the divergence of stochastic trajectories using real gauges we have explored a previously untested gauge freedom resulting from the choice of a non-square noise matrix. The resulting distribution of weights becomes highly skewed on a time scale proportional to the inverse of the mean atom number. The weight parameter for most stochastic trajectories tends towards zero,
whereas very few tend towards a large weight. Such distributions are likely to be ubiquitous for unitary real-time stochastic-gauge simulations with real gauges, as the weight distribution necessary broadens with time while the mean weight must remain unity.

While such skewed distributions are difficult to sample with the usual stochastic methods, they are ideally suited to Monte Carlo importance sampling techniques that preferentially sample high-weight trajectories. Indeed we found enormous improvements over stochastic sampling using both the Metropolis and branching algorithms. The branching algorithm is the more straightforward to apply because it has only one free parameter (the branching interval) and produces results at every time step. We suggest it as the best starting point for future Monte Carlo simulations. By contrast the Metropolis algorithm has to be targeted to a particular time and so seems less useful. However, there is a lot more freedom in the Metropolis algorithm and a vast literature exists on optimising sampling for particular distribution. Thus it seems quite possible that it will be better suited to some problems, especially when further improvements over the branching algorithm are desirable.

Traditionally Monte Carlo techniques have been highly successful in imaginary-time calculations for thermal equilibrium. This paper has extended the use of these techniques to real-time quantum-dynamical calculations and thus opens a new domain of application for these algorithms. In future, these techniques need to be extended to many-mode, many-particle problems where exact solutions are not known.

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