First-principles Quantum Simulations of Many-mode Open Interacting Bose Gases Using Stochastic Gauge Methods

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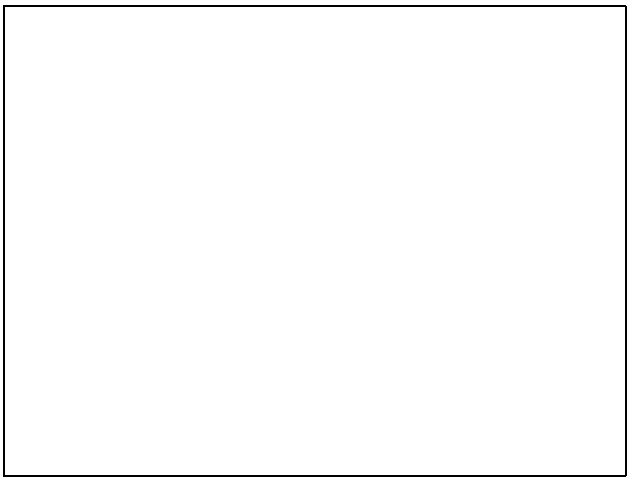

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Statement of Originality

Except where acknowledged in the customary manner, the material presented in this thesis is, to the best of my knowledge and belief, original and has not been submitted in whole or in part for a degree in any university.

Piotr P. Deuar

Peter D. Drummond

Statement of Contribution by Others

The original concepts of the gauge P representation and of (drift) stochastic gauges were due to Peter Drummond, as was the suggestion to investigate boundary term removal and thermodynamics of uniform 1D gases. The concepts in Section 5.7 and Subsection 6.1.4, are also due to Peter Drummond, but are included because they are important for a background understanding.
The XMDS program [http://www.xmds.org/] (at the time, in 2001, authored by Greg Collecutt and Peter Drummond) was used for the calculations of Chapter 6, while the calculations in the rest of the thesis were made with programs written by me but loosely based on that 2001 version of XMDS.
The exact Yang & Yang solutions in Figure 11.10 were calculated with a program written by Karen Kheruntsyan.

Piotr P. Deuar

Peter D. Drummond

Acknowledgements

Above all I thank Prof. Peter Drummond, my principal Ph.D. supervisor. You led by example, and showed me what true scientific work is all about — along with the sheer glee of it. Our many physics discussions were always extremely illuminating and productive. Thank you for your patience (which I hope not to have stretched too thin) and positive attitude.

I also owe much to Drs. Bill Munro and Karen Kheruntsyan, my secondary supervisors in the earlier and later parts of my candidature, respectively. Your assistance through this whole time has been invaluable. I would also like to thank Dr. Margaret Reid, who first introduced me to real scientific work in my Honours year.

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More personally, I thank my wife Maria, for her support and above all her extreme tolerance of the husband engrossed in physics, particularly while I was writing up.

Publications by the Candidate Relevant to the Thesis but not forming part of it

Some of the research reported in this thesis has been published in the following refereed publications:

1. P. Deuar and P. D. Drummond. Stochastic gauges in quantum dynamics for many-body simulations. *Computer Physics Communications* **142**, 442–445 (Dec. 2001).

2. P. Deuar and P. D. Drummond. Gauge P-representations for quantum-dynamical problems: Removal of boundary terms. *Physical Review A* **66**, 033812 (Sep. 2002).

3. P. D. Drummond and P. Deuar. Quantum dynamics with stochastic gauge simulations. *Journal of Optics B — Quantum and Semiclassical Optics* **5**, S281–S289 (June 2003).

4. P. D. Drummond, P. Deuar, and Kheruntsyan K. V. Canonical Bose gas simulations with stochastic gauges. *Physical Review Letters* **92**, 040405 (Jan. 2004).

This is noted in the text where appropriate.

Abstract

The quantum dynamics and grand canonical thermodynamics of many-mode (one-, two-, and three-dimensional) interacting Bose gases are simulated from first principles. The model uses a lattice Hamiltonian based on a continuum second-quantized model with two-particle interactions, external potential, and interactions with an environment, with no further approximations. The interparticle potential can be either an (effective) delta function as in Bose-Hubbard models, or extended with a shape resolved by the lattice.

Simulations are of a set of stochastic equations that in the limit of many realizations correspond exactly to the full quantum evolution of the many-body systems. These equations describe the evolution of samples of the gauge P distribution of the quantum state, details of which are developed.

Conditions under which general quantum phase-space representations can be used to derive stochastic simulation methods are investigated in detail, given the criteria: 1) The simulation corresponds exactly to quantum mechanics in the limit of many trajectories. 2) The number of equations scales linearly with system size, to allow the possibility of efficient first-principles quantum mesoscopic simulations. 3) All observables can be calculated from one simulation. 4) Each stochastic realization is independent to allow straightforward use of parallel algorithms. Special emphasis is placed on allowing for simulation of open systems. In contrast to typical Monte Carlo techniques based on path integrals, the phase-space representation approach can also be used for dynamical calculations.

Two major (and related) known technical stumbling blocks with such stochastic simulations are instabilities in the stochastic equations, and pathological trajectory distributions as the boundaries of phase space are approached. These can (and

often do) lead to systematic biases in the calculated observables. The nature of these problems are investigated in detail.

Many phase-space distributions have, however, more phase-space freedoms than the minimum required for exact correspondence to quantum mechanics, and these freedoms can in many cases be exploited to overcome the instability and boundary term problems, recovering an unbiased simulation. The stochastic gauge technique, which achieves this in a systematic way, is derived and heuristic guidelines for its use are developed.

The gauge P representation is an extension of the positive P distribution, which uses coherent basis states, but allows a variety of useful stochastic gauges that are used to overcome the stability problems. Its properties are investigated, and the resulting equations to be simulated for the open interacting Bose gas system are derived.

The dynamics of the following many-mode systems are simulated as examples: 1) Uniform one-dimensional and two-dimensional Bose gases after the rapid appearance of significant two-body collisions (e.g. after entering a Feshbach resonance). 2) Trapped bosons, where the size of the trap is of the same order as the range of the interparticle potential. 3) Stimulated Bose enhancement of scattered atom modes during the collision of two Bose-Einstein condensates. The grand canonical thermodynamics of uniform one-dimensional Bose gases is also calculated for a variety of temperatures and collision strengths. Observables calculated include first to third order spatial correlation functions (including at finite interparticle separation) and momentum distributions. The predicted phenomena are discussed.

Improvements over the positive P distribution and other methods are discussed, and simulation times are analyzed for Bose-Hubbard lattice models from a general perspective. To understand the behavior of the equations, and subsequently optimize the gauges for the interacting Bose gas, single- and coupled two-mode dynamical and thermodynamical models of interacting Bose gases are investigated in detail. Directions in which future progress can be expected are considered.

Lastly, safeguards are necessary to avoid biased averages when exponentials of Gaussian-like trajectory distributions are used (as here), and these are investigated.

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Thesis Rationale and Structure

Rationale

It is a common view that first-principles quantum simulations of mesoscopic dynamics are intractable because of the complexity and astronomical size of the relevant Hilbert space. The following quotes illustrate the significance of the problem: include[4, 5]:

> *"Can a quantum system be probabilistically simulated by a classical universal computer? . . . the answer is certainly, No!"* (Richard P. Feynman, 1982).
>
> *"One is forced to either simulate very small systems (i.e. less than five particles) or to make serious approximations"* (David M. Ceperley, 1999).

This is certainly true if one wishes to follow all the intricate details of a wavefunction that completely specifies the state of the system. Hilbert space size grows exponentially as more subsystems (e.g. particles or modes) are added, and methods that calculate state vectors or density matrix elements bog down very quickly. Path integral Monte Carlo methods also fail because of the well-known destructive interference between paths that occurs when one attempts dynamics calculations.

Such a situation appears very unfortunate because for many complex physical systems a reliable simulation method is often the only way to obtain accurate quantitative predictions or perhaps even a well-grounded understanding. This is particularly so in situations where several length/time/energy scales or processes are of comparable size/strength, or when non-equilibrium phenomena are important.

The need for reliable quantum dynamics simulations can be expected to become ever more urgent as more mesoscopic systems displaying quantum behavior are accessed experimentally. A pioneering system in this respect are the Bose-Einstein condensates of alkali-atom gases realized in recent years[6, 7, 8, 9].

There is, however, a very promising simulation method using phase-space representations that works around this complexity problem. In brief, a correspondence is made between the full quantum state and a distribution over separable operator kernels, each of which can be specified by a number of variables *linear* in the number of subsystems (e.g. modes). If one then samples the operator kernels according to their distribution, then as the number of samples grows, observable averages of these operators approach the exact quantum values, i.e. "emerge from the noise". In principle one could reach arbitrary accuracy, but in practice computer power often severely limits the number of samples. Nevertheless, if one concentrates only on bulk properties, and is prepared to sacrifice precision beyond (typically) two to four significant digits, many first-principles quantum mesoscopic dynamics results can be obtained. The mesoscopic region can be reached because simulation time scales only log-linearly[1] ($N_{\rm var} \log N_{\rm var}$) with variable number $N_{\rm var}$, and so still scales log-linearly with system size. Some initial examples of calculations with this method, particularly with the positive P representation[10, 11] based on a separable coherent state basis, are many-mode quantum optics calculations in Kerr dispersive media[12, 13] evaporative cooling of Bose gases with repulsive delta-function interactions[14, 15], and breathing of a trapped one-dimensional Bose gas[1].

In summary, first-principles mesoscopic quantum dynamics is hard, but some progress can (and has) been made in recent years. In broad terms, *the aim of the work reported in this thesis is to advance the phase-space simulation methods some more* . The investigation here is carried out in several directions:

[1]This is because discrete Fourier transforms, usually required for kinetic energy evaluation, can be calculated on timescales proportional to $N_{\rm var} \log N_{\rm var}$. For some particularly demanding models, the scaling may be log-polynomial in $N_{\rm var}$ due to an increased number of terms in the equation for each variable if there is complicated coupling between all subsystem pairs, triplets, etc. In any case, simulation time never scales exponentially, as it would for brute force methods based on density matrix or state vector elements.

1. **Stochastic gauges** Many phase-space distributions have more phase-space degrees of freedom than the minimum required for exact correspondence to quantum mechanics. Each such degree of freedom leads to possible modifications of the stochastic equations of motion by the insertion of arbitrary functions or *gauges* in an appropriate way. While the choice of these gauge functions does not influence the correspondence to quantum mechanics in the limit of infinitely many samples, it can have an enormous effect on the efficiency and/or statistical bias of a simulation with a finite number of samples. (Hence the use of the word "gauge", in analogy with the way electromagnetic gauges do not change the physical observables but can have an important effect on the ease with which a calculation proceeds). In particular, non-standard choices of these gauge functions can lead to enormous improvements in simulation efficiency, or can be essential to allow any unbiased simulation at all.

   Here, a systematic way to include these freedoms is derived and ways of making an advantageous gauge choice are considered in some detail. As a corollary, some results present in the literature[2, 1, 3] are found to be examples of non-standard gauge choices.

   The gauge P representation, which is a generalization of the successful positive P representation based on a coherent state basis to allow a variety of useful gauges, is explained. Application of it to interacting Bose gases is developed.

2. **Removal of systematic biases using stochastic gauges**. Two major (and related) stumbling blocks for phase-space distribution methods have been instabilities in the stochastic equations, and pathological trajectory distributions as the boundaries of phase space are approached. These occur for nonlinear systems and can (in fact, apart from special cases, *do*) lead to overwhelming noise or systematic biases in the calculated observables, preventing dependable simulations. To date this has been "problem number one" for these methods.

   In this thesis it is shown how appropriate stochastic gauges can be used to overcome the instability and boundary term problems in a wide range of models, recovering an unbiased simulation, and opening the way for reliable simula-

tions. Heuristic ways of achieving this in general cases are considered in detail, and examples are given for known cases in the literature.

3. **Improvement of efficiency using stochastic gauges** The stochastic gauge method also has the potential to significantly improve the efficiency of simulations when appropriate gauges are chosen. In particular, the time for which useful precision is obtained can be extended in many cases by retarding the growth of noise. This is investigated for the case of gauge P simulations of interacting Bose gases and some useful gauges obtained. The regimes in which improvements can be seen with the gauges developed here are characterized. Heuristic guidelines for gauge choice in more general representations and models are also given. Example simulations are made.

4. **General requirements for usable distributions in open systems** Another aim here is to determine what are the bare necessities for a phase-space distribution approach to be successful, so that other details of the representation used (e.g. choice of basis) can be tailored to the model in question. This can be essential to get any meaningful results, as first-principles mesoscopic simulations are often near the limit of what can be tractably calculated. To this end, general features of the correspondence between quantum mechanics and stochastic equations for the variables specifying the operator kernels are considered in some detail.

   Particular concern is given to simulating open systems, as most experimentally realizable systems do not exist in isolation and will have significant thermal and also particle-exchange interactions with external environments. These must usually be taken into account for an accurate description. (The alternative is to make wholesale approximations to the model whose precise effect is often difficult to ascertain).

5. **Application to thermodynamic calculations** A separate issue are static calculations of thermodynamic equilibrium ensembles. These have traditionally been the domain of quantum Monte Carlo methods, the most versatile

of which have been those based on the path integral approach. While path integral methods are generally not useful for dynamical calculations because destructive interference between the paths occurs extremely rapidly, masking any dynamics, good results can be obtained for static thermodynamic ensemble calculations. If the model is kind, even $\mathcal{O}(10^4)$ particles or modes can be successfully simulated, if one again concentrates on bulk properties and only several significant digits.

Phase-space representations that include dynamically changing trajectory weights can also be used for thermodynamics calculations. The thermal density matrix is evolved with respect to inverse temperature after starting with the known high temperature state. (Such simulations are sometimes said to be "in imaginary time" because of a similarity between the resulting equations and the Schrödinger equation after multiplying time by i). This approach appears competitive with path integral Monte Carlo methods in terms of efficiency, but offers two distinct advantages: Firstly, all observables can in principle be calculated in a single simulation run, which is not the case in path integral methods. These latter require separate algorithms for e.g. observables in position space, momentum space, or observables not diagonal in either. Secondly, a single simulation run gives results for a range of temperatures, while in path integral methods a new simulation is needed for each temperature value.

6. **Demonstration with non-trivial examples** Lastly, but perhaps most importantly, one wishes to demonstrate that the results obtained actually are useful in non-trivial cases. Simulations of dynamics and thermodynamics in a variety of mesoscopic interacting systems are carried out, and their physical implications considered. The emphasis will be foremost on simulations of interacting Bose gases. It is chosen to concentrate on these because they are arguably the systems where quantum effects due to collective motion of atoms are most clearly seen and most commonly investigated by contemporary experiments. This refers, of course, to the celebrated Bose-Einstein condensate experiments on cold, trapped, rarefied, alkali-metal gases. (For a recent

overview see, for example, the collection of articles in Nature *Insight on ultracold matter*[16, 17, 18, 19, 20].) As these gases are an extremely dynamic field of research the need for first-principle simulation methods appears urgent here.

The "holy grail" of quantum simulations, which would be a universally-applicable black-box tractable simulation method[2], probably does not exist. However, simulations are of such fundamental importance to reliable predictions in mesoscopic physics that any significant progress has the potential to be a catalyst for far-ranging discoveries (and in the past often has).

Structure

This thesis begins with two introductory chapters, which explain in more detail the background issues. That is, Chapter 1 discusses the fundamentals of why many-body quantum simulations are difficult, compares several approaches, and motivates the choice to work on the mode-based phase-space representation simulation methods considered in this thesis. Chapter 2 summarizes the interacting Bose gas model that will be considered in all the simulation examples, and discusses under what circumstances a first-principles rather than a semiclassical calculation is needed to arrive at reliable predictions.

The body of the thesis is then divided into three parts of a rather different nature. Part A investigates what general properties of a phase-space representation are needed for a successful simulation, and explains the gauge P representation, which will be used in later parts. Part B calibrates this method on some toy problems relevant to the interacting Bose gas case, while Part C applies them to non-trivial mesoscopic systems (dynamics and thermodynamics of interacting Bose gases).

Accordingly, Chapter 3 presents a generalized formalism for phase-space representations of mixed quantum states and characterizes the necessary properties for an exact correspondence between quantum mechanics and the stochastic equations.

[2]In Newtonian dynamics this is just the usual "start with initial conditions and integrate the differential equations".

The stochastic gauge technique, which forms the basis of the rest of the developments in this thesis, is developed in Chapter 4. In Chapter 5, properties of the gauge P representation are investigated, and its application to interacting Bose gases developed. In Chapter 6 it is explained how stochastic gauges can be used to overcome "technical difficulty number one": the systematic "boundary term" biases that otherwise prevent or hinder many attempted phase-space distribution simulations. Some relevant technical issues regarding stochastic simulations have been relegated to Appendices.

One- and two-mode toy models are used in Part B to check correctness of the method, and to optimize the gauge functions in preparation for the target aim of simulating multi-mode systems. These models are the single-mode interacting Bose gas dynamics in Chapter 7, the dynamics of two such Rabi-coupled modes in Chapter 8, and grand canonical single-mode thermodynamics in Chapter 9.

Finally, Chapters 10 and 11 give examples of nontrivial many-mode simulations of many-mode interacting Bose gas dynamics and grand canonical thermodynamics, respectively.

Chapter 12 summarizes and concludes the work along with some speculation on fruitful directions of future research.