Chapter 12

Conclusions

12.1 Overview of main results

As with the thesis, the main results obtained can be divided into three parts:

1. **Theoretical background work regarding general phase-space distributions**. The first aim here has been to specify what freedoms are available to the broadly conceived phase-space distribution approach when it is to be used for first-principles simulations of mesoscopic quantum mechanics. The considerations of Chapter 3 led to a set of necessary requirements for any useful simulation, summarized in Section 3.6. Some fundamental expressions (e.g. observable estimators) have been given for general representations (i.e. choices of kernel). The usefulness of a given representation (which is closely related to basis choice) is highly system dependent, and so it is hoped that the results and considerations of Chapter 3 will aid in matching representations to problems.

   With a given representation, often there still remains a wide range of stochastic equations that simulate the same physical problem, but strongly differ in efficiency. The stochastic gauge formalism developed in Chapter 4 describes the freedoms available in a systematic way. At the coarsest level there are two main kinds: Those that arise when making the correspondences from master to Fokker-Planck equations (kernel gauges), and from Fokker-Planck to

stochastic equations (diffusion gauges). Some analysis of these freedoms for general gauge choices has also been made. Uses have been found to include

(a) Improvement of efficiency by tailoring the shape of the distribution of random variables to improve sampling.

(b) Removal of biases due to a broad class of so-called boundary term errors, which are due to instabilities or divergences in the stochastic equations.

(c) Allowance for calculations of grand canonical ensemble properties by the inclusion of a dynamically varying (with simulation steps) weight.

Part of the freedoms (e.g. real diffusion gauges) have been determined to not be useful. The stochastic gauge formalism includes in a systematic way several recent developments[2, 1, 65, 3, 66, 56, 61] as special cases. A relatively restricted set of gauges that still allows the uses listed above has been identified in Section 4.5 as the "standard gauges".

The causes and symptoms of boundary term errors (sampling biases that do not abate in the infinite sample number limit), have been considered in considerable detail in Chapter 6. These have been major obstacles for many phase-space simulations in the past. Two kinds of processes have been identified as causing these — either arising when making the correspondence between master and Fokker-Planck equations (first kind), or when calculating observable estimates using the simulated random variables (second kind). Several warning symptoms of these errors, which can be identified by inspection of the stochastic equations prior to simulation, have been identified.

It has been found that appropriate choices of drift stochastic gauges (a class of Kernel gauge) can be used to remove the biases and instabilities in many (or possibly all) cases of boundary term errors of the first kind. This is demonstrated in several simple examples where boundary term errors have been known to occur, and also used in some subsequent many-mode calculations where required. Heuristic guidelines for appropriate gauge choice have been found and given in Section 6.3.2.

2. **Investigation of gauge P representation and development of gauges for use with interacting Bose gases**. This representation is an extension of the successful positive P representation based on coherent states. The added complex weight factor is shown to allow the use of the standard gauges to improve simulations, remove possible boundary term bias, and extend the range of physical models that can be simulated (thermodynamic calculations).

   The emphasis here has been almost exclusively on simulations of open Bose gases with binary interactions. Equations for dynamics and thermodynamics calculations have been obtained (including non-delta-function interparticle potentials). Part B searched for useful choices of gauges for dynamics and thermodynamics calculations, given the constraint that they be local (i.e. dependent only on variables at a single lattice point). This constraint is not optimal, but is a basic starting point for possible further investigation. Both diffusion and drift gauges that improve simulations under appropriate conditions were found. Diffusion gauges were able to significantly improve sampling and useful simulation times in dynamics calculations, while drift gauges are essential for any accurate thermodynamic calculation, and were found to also give sampling improvement in dynamics under some conditions (See Chapter 8).

   Analyses were made of the expected behavior of multi-mode simulations, and subsequently confirmed in the actual calculations. In dynamics calculations, simulation time is found to be limited by properties of the most highly occupied lattice point, and a robust estimate of this time for positive P simulations is given by (10.4). Relative to this positive P simulation time, it was found that simulation time improvement with diffusion gauges occurs when lattice spacing is greater than the healing length in the gas. Local drift gauges were found to give even more improvement in simulation time but for a much narrower range of systems in which two-body collision effects dominate kinetic processes, as in some simulations in Chapter 8. Thermodynamic simulations were made possible with judicious use of a drift gauge. It was also found that

simulation precision at a target temperature and chemical potential was dependent (sometimes strongly) on the (otherwise free) choice of chemical potential at higher temperatures.

3. **Simulations of many-mode interacting Bose gases** Several nontrivial mesoscopic systems of open interacting Bose gases have been simulated. These were dynamics of:

   - Uniform 1D and 2D gas with effectively local scattering. Wave behavior occurring in the two- or three-particle correlations (but not density) was found, and displays some interesting properties (e.g. movement of main wavefront at $\sqrt{2}$ the speed of sound).
   - Uniform 1D gas with extended nonlocal interparticle interactions. Correlation wave behavior was also seen, but with different properties than for the locally-interacting gas. Simulation time was found to increase significantly with respect to a locally-interacting gas with the same interaction energy density.
   - Trapped 1D gas with extended interactions on the length scale of the trap. Strong interplay between the scattering and breathing of the atom cloud in the trap was seen.
   - Scattering of atoms from colliding BECs in 3D. Bosonic enhancement of initially empty modes was seen in a physical situation similar to the Vogels *et al* four wave mixing experiment[41] (the difference was that there were less atoms in the simulation). Additionally, a significant suppression of the spontaneous scattering process compared to the imaginary scattering length estimate is predicted.

   Also:

   - Calculations of grand canonical ensembles were made for the uniform 1D gas at temperature T and chemical potential μ. Physical regimes reached included the nondegenerate strongly interacting fermionized regime, and the quantum degenerate decoherent regime. Spatial correlation functions

of first $\overline{g}^{(1)}(x)$, second $\overline{g}^{(s)(x}$ and third order $\overline{g}^{(3)}(x,y)$ have been calculated as well as momentum distributions. A transition regime where enhanced atom pairing occurs at a preferred interparticle distance has been found. This occurs when the de Broglie thermal wavelength λ_T is of the same order as the 1D scattering length $a_{1\mathrm{D}}$ (effectively the "size" of the atom for scattering processes). The pairing was found to occur at distances $\approx \lambda_T/2$ for the parameters simulated.

These simulations can be tractable even with very large numbers of modes or particles in the system given the right conditions, as evidenced by Section 10.7, where there were 1009 152 lattice points and 150 000 atoms on average.

Situations where there are several length scales of similar order, or processes of similar strength are of particular interest for first-principles simulations because it is difficult to make accurate quantitative predictions otherwise. The calculations in Sections 10.6 and 10.7 and the thermodynamics calculations were of this type, and were seen to be amenable to simulation using the gauge P method. In fact, even in a perturbative regime (e.g. the correlation phenomena at low intensity can probably be treated by Bogoliubov approximation approach), the equations are convenient to use: One simply repeatedly simulates a GP equation with noise and takes appropriate averages. All quantum effects are included to within statistical precision. The caveat is that simulation time is limited. Nevertheless, many phenomena can still be seen, and simulation time can be extended with appropriate gauges under some conditions.

12.2 Future directions of improvement

The local diffusion gauges developed here give significant improvements only when the lattice is relatively sparse, and/or scattering interactions are dominant. A way to overcome these limitations might be found by using nonlocal diffusion gauges that would depend on neighboring, or preferably all, lattice amplitudes $\alpha_{\mathbf{n}}$, $\beta_{\mathbf{n}}$. A possible starting point would be to consider optimizing diffusion gauges in the

opposite regime of strong kinetic interactions and weak scattering. The equations for such a model are probably best considered in Fourier space where kinetic processes take on a simpler form.

Another major issue is the reduction of simulation time with system size due to increasing weight or z_0 spread when drift gauges are used. (As was discussed in Section 10.2.4). A starting point here may be to determine why the lattice-dependent diffusion gauge (10.26) did not give the expected simulation time improvements (10.28). If the expected $M^{-1/4}$ scaling could be achieved, many useful mesoscopic simulations should become accessible with a drift gauge. Such a drift-gauged simulation would be free of moving singularities, and possibly also extend simulation time as was seen for the drift gauged one- and two-mode systems.

A completely different but potentially very promising approach is to use non-coherent state kernels for the representation. Certainly in many low temperature regimes this would be a more efficient approach if viable representations could be found because the low temperature ground and low excited states are often far from coherent states. Some preliminary attempts with squeezed state kernels give mixed results[104].

For thermodynamics calculations of properties at and around a target temperature and chemical potential, an important outstanding issue is to characterize the influence of the choice of $\mu(T)$ at intermediate temperature values. It is conceivable that a good choice of $\mu(T)$ may give dramatic improvement in precision and significantly extend the physical region that can be simulated. Some precision and simulation time improvement should also be obtained by using a more sophisticated importance sampling technique than the rough method used in Chapter 11. Some preliminary results indicate that using a Metropolis sampling algorithm[105] extends the reachable γ, $\widetilde{T}$ regime[106].