

**Towards  
FULLY  
QUANTUM  
MANY-BODY  
Simulations of  
BOSE-EINSTEIN  
CONDENSATES**

*Piotr Deuar and Peter D. Drummond*

31 March 2002

- A many body simulation with no semiclassical approximations can allow or improve the investigation of quantum-mechanical effects involving many modes.  
**e.g. correlations, quantum phase changes, fluctuations, non-equilibrium behaviour.**
- *Many body-simulations are notoriously difficult because of the rapid growth of Hilbert space with number of bodies.*
- “Can a quantum system be probabilistically simulated by a classical universal computer? . . . If you take the computer to be the classical kind . . . the answer is certainly, No!” (Richard P. Feynman *Simulating Physics with Computers*)

# Quantum model of a BEC

Neutral atoms in  $d = 1, 2, \text{or } 3$  dimensions:

$$\hat{H} = \int d^d \mathbf{x} \left[$$

$$\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger(\mathbf{x}) \nabla \hat{\Psi}(\mathbf{x})$$

Kinetic Energy, mass  $m$

$$+ V(\mathbf{x}) \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{x})$$

Trapping Potential  $V(\mathbf{x})$

$$+ \hat{\Psi}^\dagger(\mathbf{x}) \hat{R}(\mathbf{x}) + \hat{\Psi}(\mathbf{x}) \hat{R}^\dagger(\mathbf{x})$$

Loss at Boundaries at rate  $\propto \text{Tr}[R(\mathbf{x})]$

$$+ \frac{1}{2} \int d^d \mathbf{y} U(\mathbf{x} - \mathbf{y}) \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}^\dagger(\mathbf{y}) \hat{\Psi}(\mathbf{y}) \hat{\Psi}(\mathbf{x})$$

Boson-Boson Interaction  $U(\mathbf{x} - \mathbf{y})$ .

]

# Efficiency of Numerical Methods

For  $M$  modes,  $E$  significant eigenstates per mode.

Method	Number of Complex Equations	Stochastic?
Direct Solution of Density Matrix	$(E^M)^2$	No
Quantum Trajectories	$E^M$	Yes
Positive P representation	$2M$	Yes
Hermitian P representation	$2M + 1$	Yes

The stochastic methods require averaging over a number of realisations to obtain physical quantities.

The P distribution methods are clearly the only practical methods for many modes.

# P representations

- Expand density matrix as a weighted sum of coherent-state-like kernels

$$\hat{\rho} = \int P(\vec{\alpha}, \vec{\beta}) \hat{\Lambda}(\vec{\alpha}, \vec{\beta}) d^{2M} \vec{\alpha} d^{2M} \vec{\beta}$$

with the weights  $P$ .

- Using identities like

$$\hat{a}^\dagger ||\alpha \rangle \langle \beta|| = \frac{\partial}{\partial \alpha} ||\alpha \rangle \langle \beta||$$

We convert Master equation (in  $\hat{a}$ ,  $\hat{a}^\dagger$ ) to equation in ( $\frac{\partial}{\partial \alpha} ||\alpha \rangle$  type of terms)

- Integrate by parts, *discarding boundary effects* to obtain an equivalent Fokker-Planck equation for  $P(\alpha, \beta, \Omega)$ .
- The evolution of  $P$  can be simulated efficiently by converting the Fokker-Planck equation to stochastic (i.e. noisy) equations in the variables like  $\alpha$ .

# Positive P representation

- Off-diagonal coherent state kernel.

$$\hat{\Lambda} = ||\vec{\alpha}\rangle\langle\vec{\beta}^*||e^{-\vec{\alpha}\cdot\vec{\beta}}$$

- Observeables? e.g.  $N_m$ : Number of particles in mode  $m$

$$\langle N_m \rangle = \langle \text{Re}[\alpha\beta] \rangle_{\text{trajectories}}$$

- Widely used.
- Can run into technical problems for low occupation numbers (see below).

# Hermitian P representation

- In-built weight and phase factor  $\Omega$ .

$$\hat{\Lambda} = ||\vec{\alpha} \rangle \langle \vec{\beta}^* || e^{\Omega - \vec{\alpha} \cdot \vec{\beta}} + ||\vec{\beta} \rangle \langle \vec{\alpha}^* || e^{\Omega^* - \vec{\alpha}^* \cdot \vec{\beta}^*}$$

- **Fixes existing problems in positive P distribution. (see below)**
- Can also be used to calculate temperature-dependent equilibrium states.
- Observeables? e.g.  $N_m$ : Number of particles in mode  $m$

$$\langle N_m \rangle = \frac{\langle \text{Re}[\alpha\beta e^{\Omega}] \rangle_{\text{trajectories}}}{\langle \text{Re}[e^{\Omega}] \rangle_{\text{trajectories}}}$$

# Stochastic Gauges

- Hermitian  $\mathcal{P}$  representation allows introduction of arbitrary functions (**GAUGES**) into the equations for  $\vec{\alpha}, \vec{\beta}$ .
- To introduce gauges, note that there are some identities like

$$\left[ \frac{\partial}{\partial \Omega} - 1 \right] ||\alpha \rangle \langle \beta|| e^{\Omega - \alpha\beta} = 0$$

So we can add any multiple of them to the master equation without changing anything.

- The multiple can be an arbitrary function, and will appear in the resulting stochastic equations as a quantity we can tailor to our needs.



## Positive P simulations

- Evaporative Cooling of a BEC was successfully simulated

[P. D. Drummond and J. F. Corney,  
Phys. Rev. A **60**, R2661 (1999)]

- up to 10,000 atoms simulated.
- Centre-of -mass motion seen. This is in contradiction with usual assumptions in much of semi-classical BEC theory, but is seen in experiments.
- Evidence of vortices seen.
- Positive P method encounters signal-to-noise ratio problems after the time of condensation.





# Problems with Previous calculations

- Most modes have a small occupation number, therefore very nonclassical behaviour.
- Positive  $P$  equations have the same form as semiclassical equations, but with noise added.
- At small occupations signal-to-noise ratio becomes small, requiring many trajectories.
- For small occupations, systematic errors may occur for very underdamped systems (As it happens, BECs have very low damping).
- Hermitian  $P$  representation can be used to fix these matters.

# One-mode analogues

- The problems at small occupation numbers are already present in a one-mode calculation.
- Finding a way to overcome the large noise and discrepancy problems for one mode, readily generalises to the many mode case.
- Problems in both cases due to only the boson-boson interaction.

# DYNAMICAL SIMULATIONS

Master Equation:

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \hat{\mathcal{L}} \{ \hat{\rho} \}$$

Form of nonlinear terms (one mode):

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{iU}{\hbar} [(\hat{a}^\dagger(\mathbf{x})\hat{a}(\mathbf{x}))^2, \hat{\rho}] + \dots$$

Form of Positive P equations:

$$\frac{\partial \alpha}{\partial t} = -2i\alpha U \alpha \beta + (1 - i)\sqrt{U} \alpha \xi(t) + \dots$$

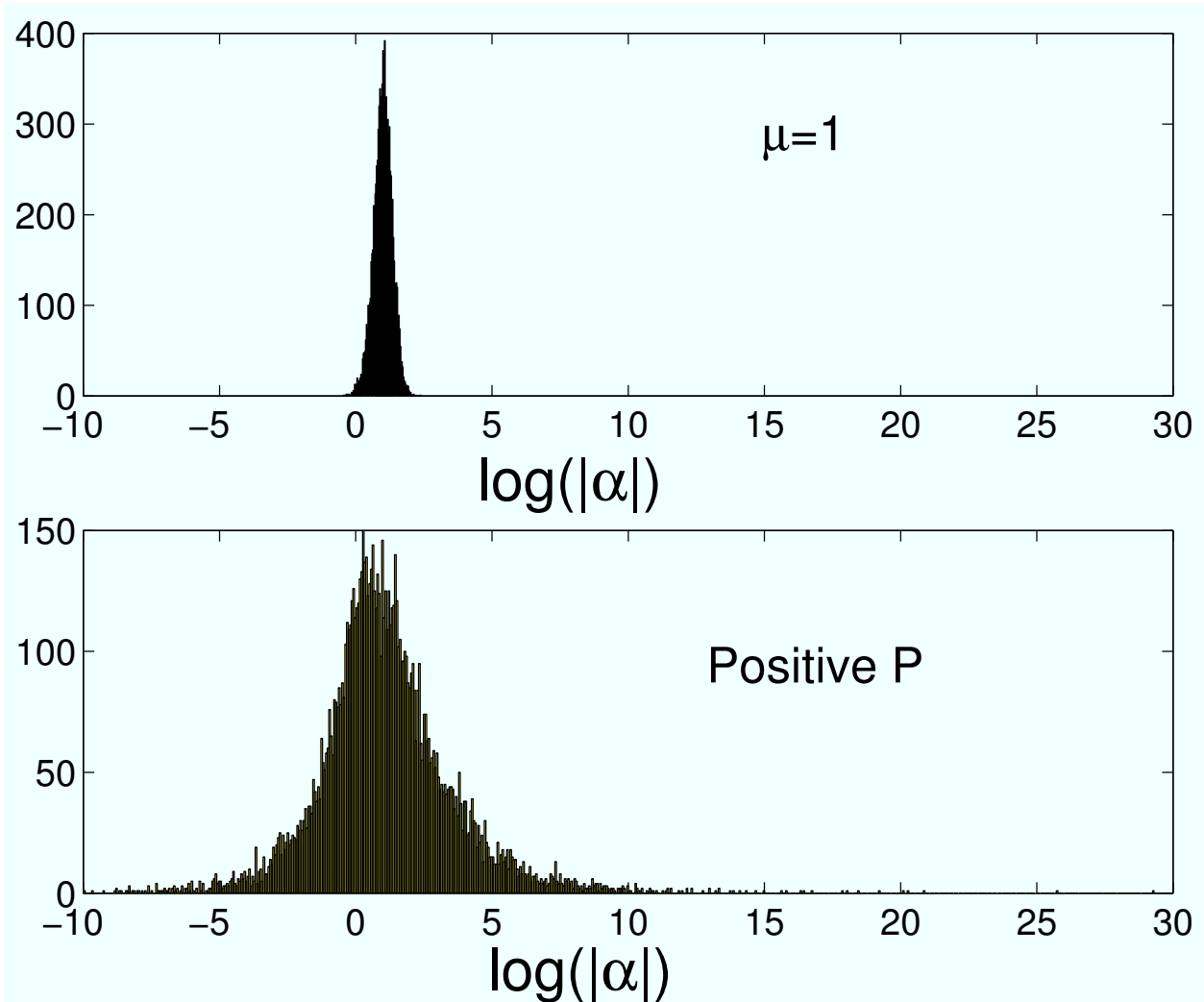
*Problem at low occupation numbers:*

**Extremely inefficient sampling of distribution by the simulated trajectories.**

After a time, some trajectories develop unstable exponential behaviour. The largest of these is so much larger than all others, that it dominates any averages performed to evaluate observables, leading to an average over effectively only that one trajectory. *The rest of the trajectories are wasted.* The nature of the problem is such that increasing the number of trajectories does not help, only changes which particular one is dominant.

*Solution:*

Introduce appropriate gauges into the  $\alpha$ ,  $\beta$ , (and the new  $\Omega$ ) equations, which remove the instability responsible for sampling breakdown.

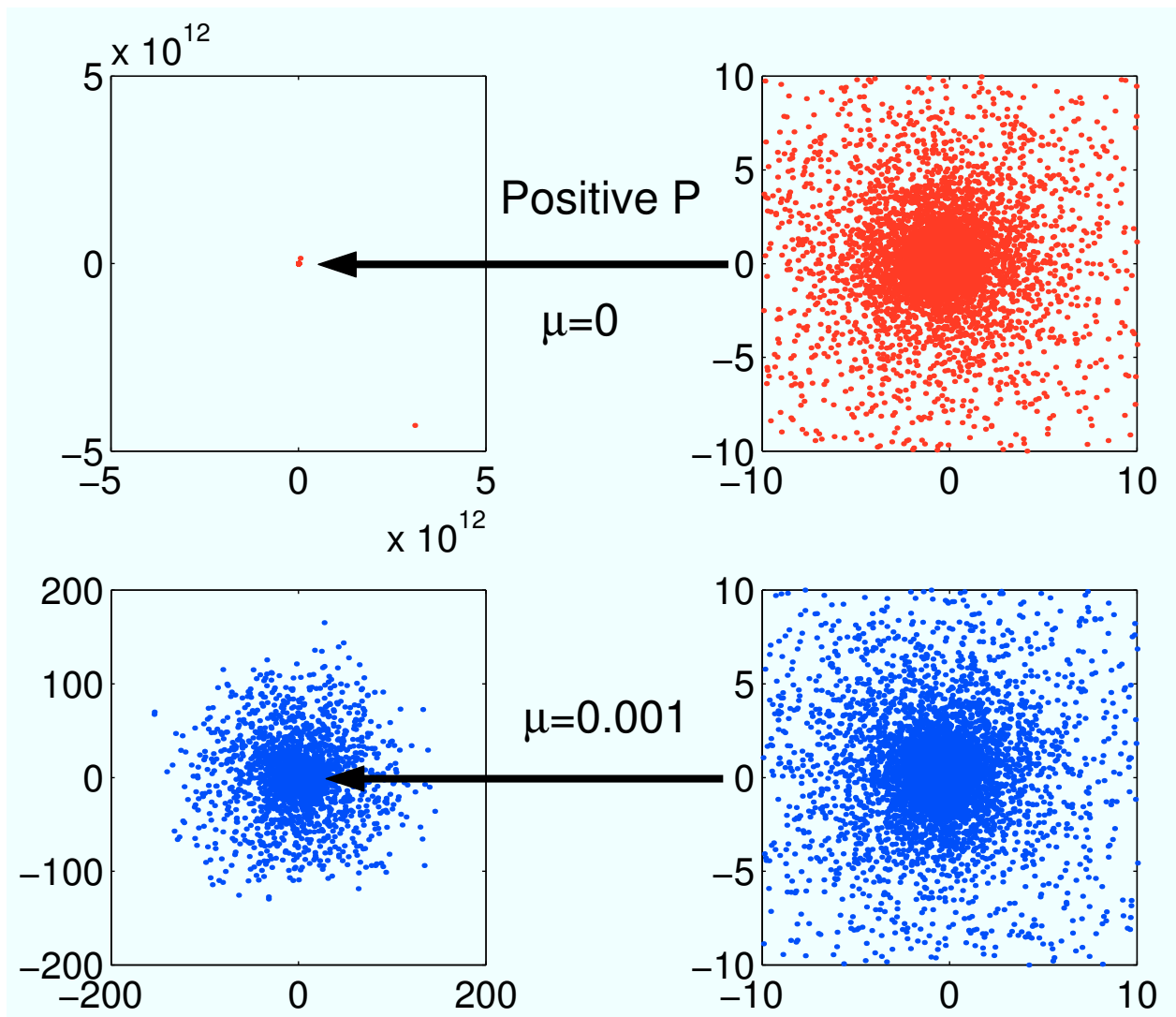


Comparison of the spread of the variable  $\alpha$  for the positive P, and a low sampling error gauge in the hermitian P representation.

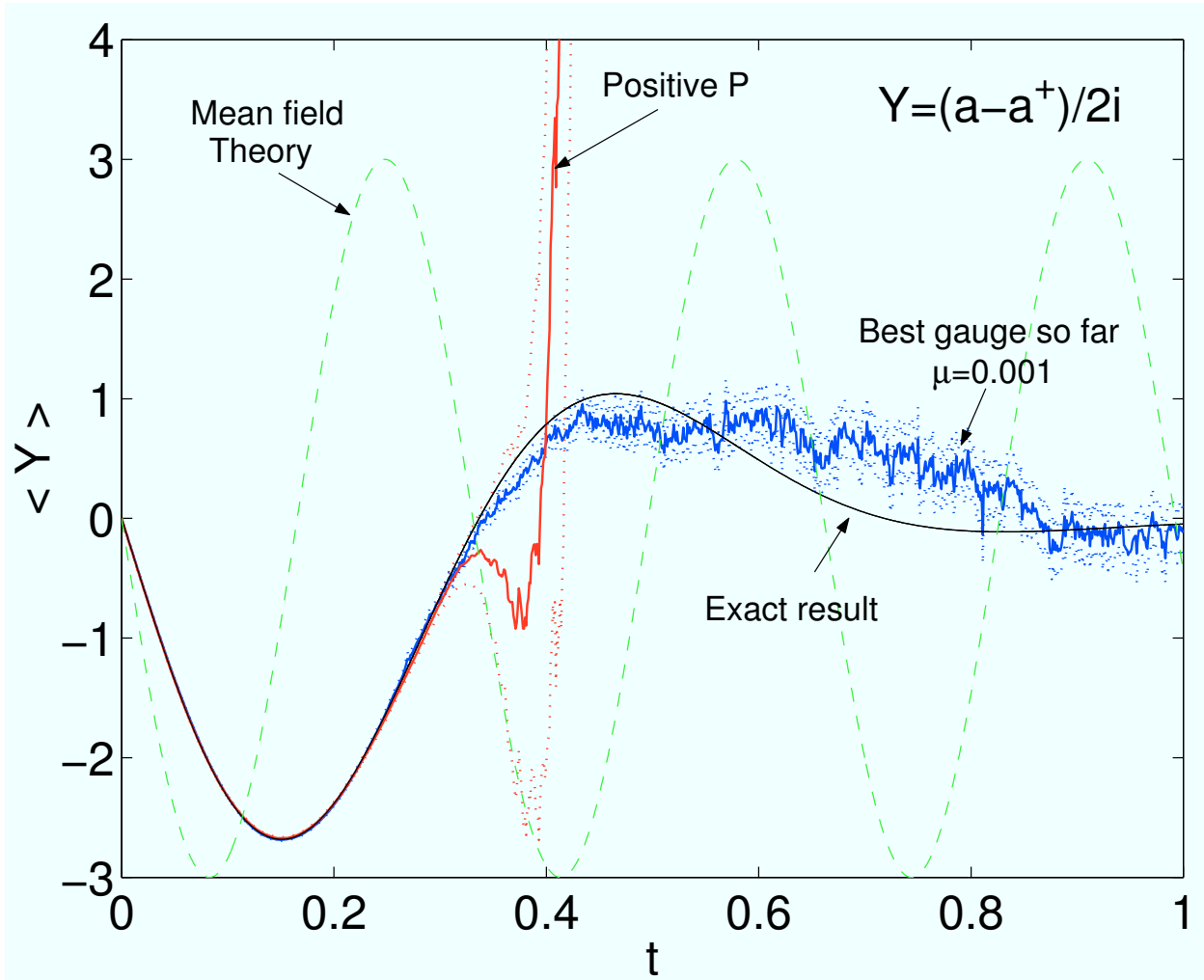
*The scale is logarithmic.*

Initial coherent state,  $U = 1$ ,  $t = 0.6$ . Note the small number of very large  $\alpha$  values in the Positive P simulation which dominate any calculated averages, making the bulk of the trajectories a waste of time to calculate. 10,000 trajectories shown.

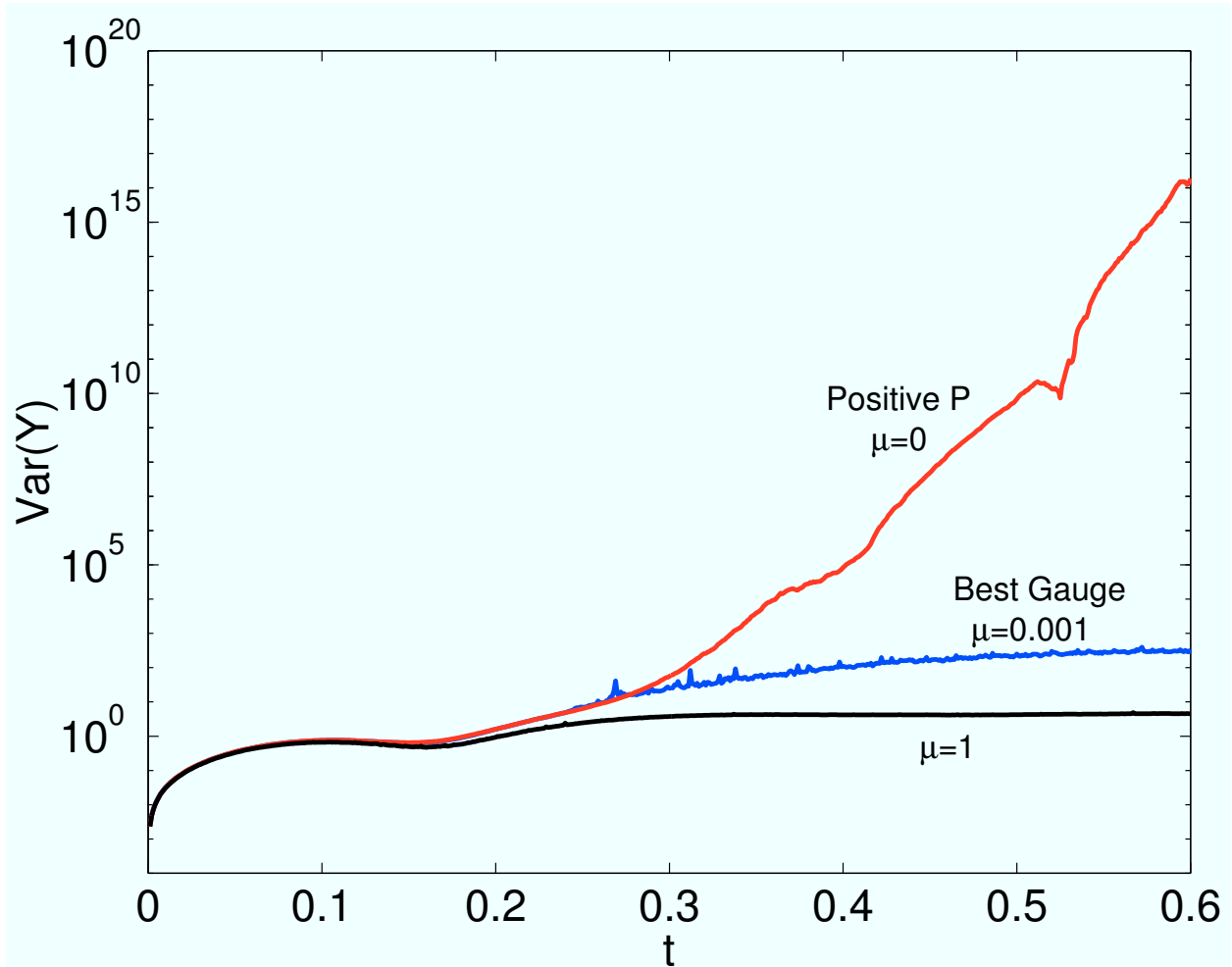




Comparison of the variable  $\alpha$  for the positive P and gauge hermitian P calculation after  $t = 0.6$ . 10,000 trajectories shown.



Comparison of simulations of the quadrature  $\hat{Y} = \frac{1}{2i}(\hat{a} - \hat{a}^\dagger)$  for an initial coherent state  $|3\rangle$  acted on by  $\hat{H} = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a})^2$ . 10,000 trajectories. Dotted lines indicate the size of the errors due to finite sampling.



Comparison of sampling errors for various stochastic simulations. Shown is the variance in quadrature  $\hat{Y}$ . Size of actual sampling uncertainty in calculated moment for  $N$  trajectories is  $\sqrt{\text{Var}(\hat{Y})/N}$ , hence number of trajectories needed for an accurate result grows as  $\text{Var}(Y)$ . **Note the logarithmic scale.**

(n.b.  $\mu$  is here is just a constant gauge parameter, not chemical potential.)

# TEMPERATURE-DEPENDENT EQUILIBRIUM STATES

- A similar Master equation approach can be used to find the temperature-dependent equilibrium states under a Hamiltonian and chemical potential  $\mu$ .
- Here the “time” variable  $\tau$  represents an inverse temperature.

$$\tau = \frac{\hbar}{k_B T}$$

- Equilibrium states for a high enough temperature ( $\tau \rightarrow 0$ ) are usually the same as for no interaction, so can be used as initial conditions, which are then advanced with  $\tau$  to obtain lower temperature equilibrium properties.

- *Must* use the Hermitian P representation because now the Master equation is for an un-normalised  $\hat{\rho}_u$ , and provision must be made for a changing weight.

Master Equation:

$$\frac{\partial \hat{\rho}_u}{\partial \tau} = -\frac{1}{2} \left[ \frac{\hat{H}}{\hbar} - \mu(\tau) \hat{N}, \hat{\rho}_u \right]_+$$

Same form as for combination of Two-photon and one-photon absorption process in real time.

Form of nonlinear terms (one mode):

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{U}{2\hbar} [(\hat{a}^\dagger(\mathbf{x})\hat{a}(\mathbf{x}))^2, \hat{\rho}]_+ + \dots$$

Form of Hermitian P equations:

$$\frac{\partial \alpha}{\partial t} = -\alpha U \alpha \beta + i\sqrt{U} \alpha \xi(t) + \frac{\mu}{2} \alpha + \dots$$

$$\frac{\partial \Omega}{\partial t} = \mu \alpha \beta + \dots$$

*Problem at low occupation numbers:*

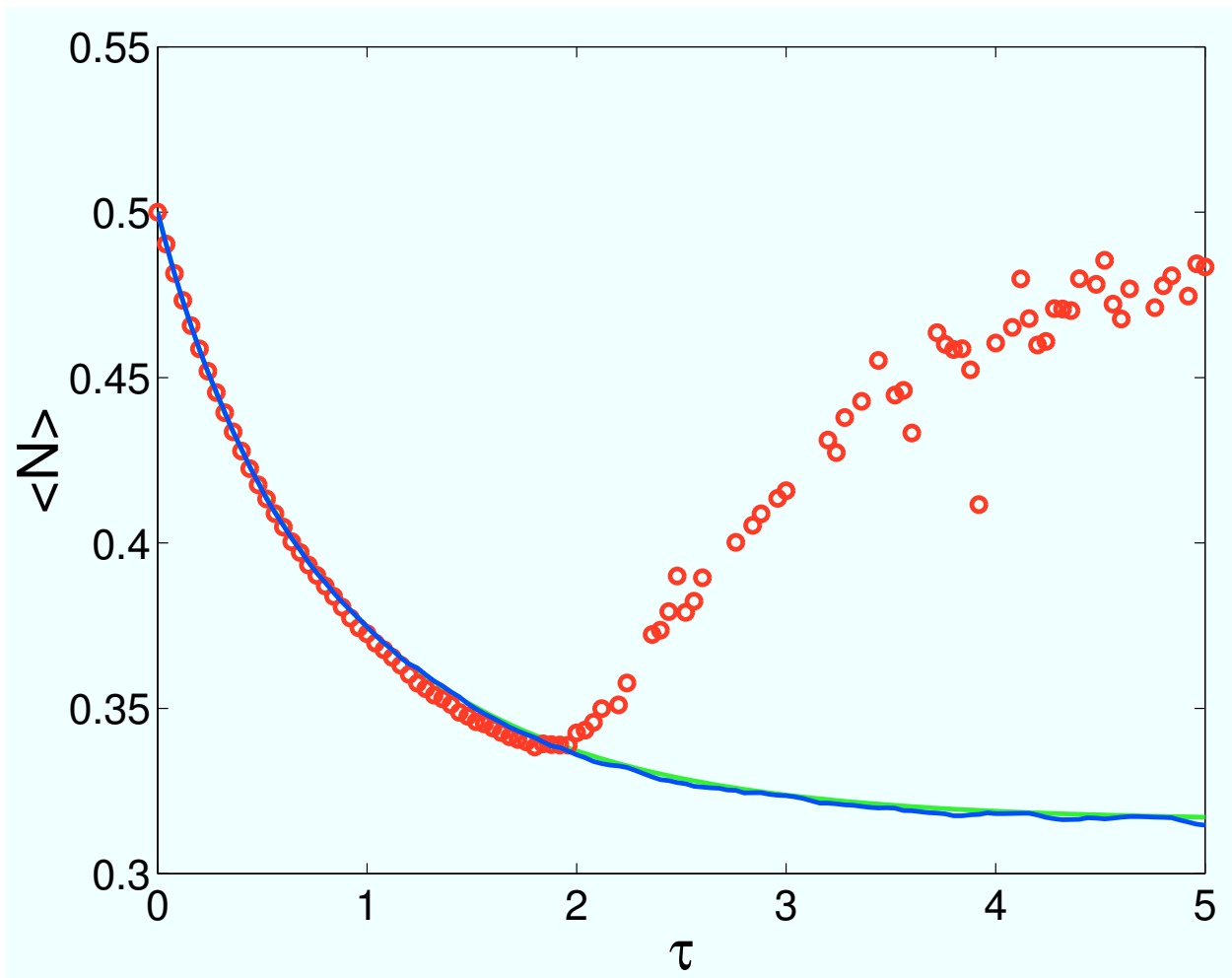
## **Systematic errors due to “phantom” trajectories**

A countable number of trajectories can escape to infinity in a **finite** time! Since their number is infinitesimal in comparison with the well-behaved trajectories they are never seen in an actual simulation. Unfortunately, because some variables may then take on infinite values, the trajectory's effect can be significant or even dominant in a calculation of observables even though its probability is zero. However, because they are never simulated, this part of the observable's value is never accumulated when averaging over trajectories. *This leads to systematic error.*

*Solution:*

Introduce appropriate gauges into the  $\alpha$ ,  $\beta$ ,  $\Omega$  equations, which prevent trajectories escaping to infinity in a finite time.

# Zero chemical potential $\mu = 0$



*Circles:* positive P simulation

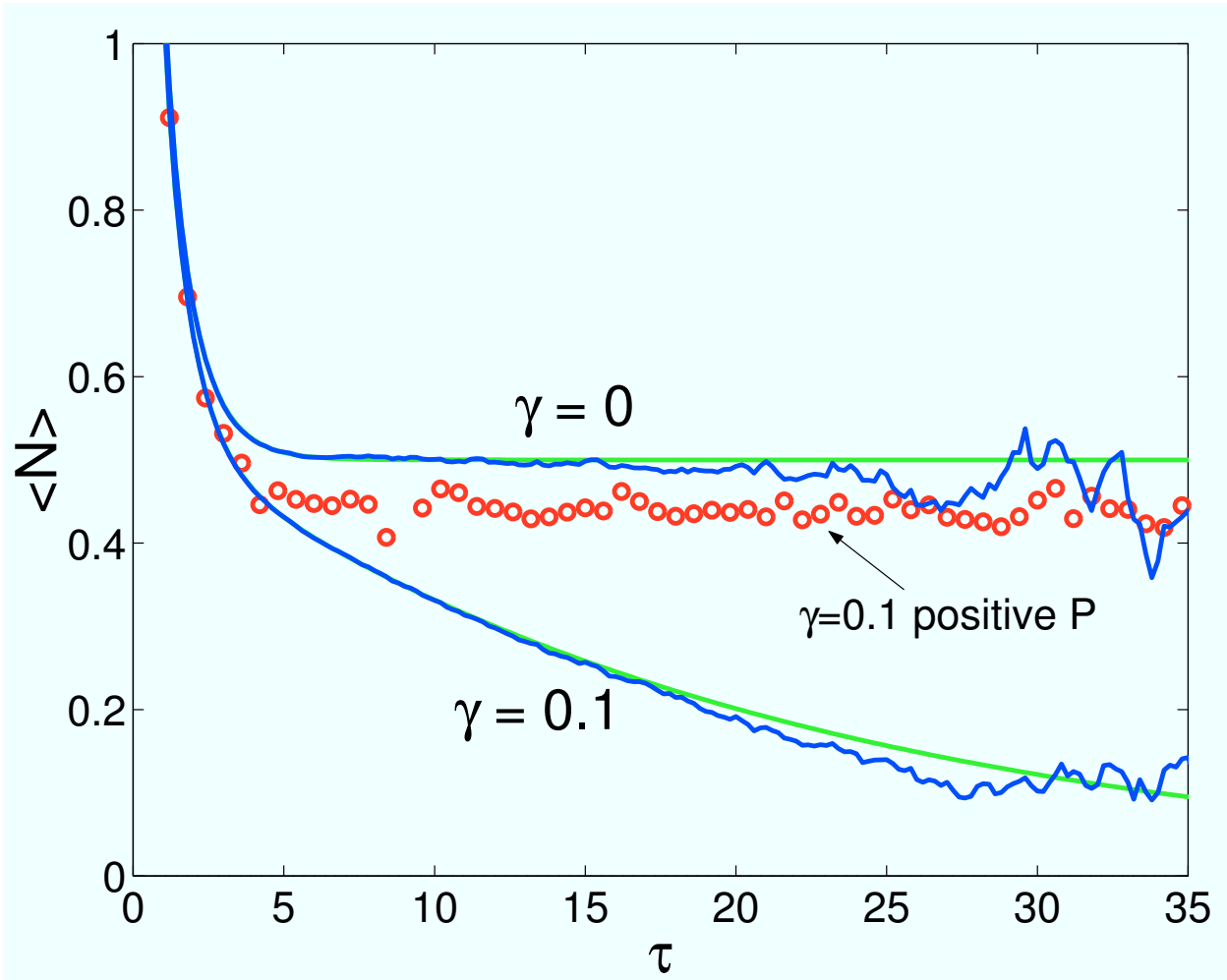
*blue line:* hermitian P gauge simulation.

*green line:* exact calculation (truncated number-state basis).

Simulation parameters: 40 000 trajectories;  
step size = 0.005;

# Non-zero chemical potential

$$\mu = -\gamma U.$$



*Circles:* positive P simulation,  $\gamma = 0.1$ ;

*blue line:* hermitian P gauge simulations;

*green line:* exact calculations (truncated number-state basis).

Simulation parameters: 100 000 trajectories; step size = 0.005;



# Conclusions

- For quantum many-body simulations, the number of equations to be solved can be made to grow only linearly with  $N$  (the number of significant subsystems) using  $P$  representation methods.
- This is far superior to direct density-matrix methods which scale exponentially.
- The problems which can occur when using the positive  $P$  representation at low occupation numbers can be overcome by using a modified version - the hermitian  $P$  representation.
- Direct first-principles simulations of Bose-Einstein condensates are currently in the process of being implemented.