Simulating the quantum dynamics of a Bose-Einstein Condensate

P. Deuar

and

P. D. Drummond

What is a BEC?

- A collection of bose atoms in which many atoms occupy the same quantum state.

- First experimentally achieved in 1995.

- Coldest known matter in the universe. ($T \approx$ 50-100 nK)

- Diffuse gas of atoms in a magneto-optical trap.

- Achieved by evaporative cooling of a gas of thermal atoms.

- Typically 1000 to 10^9 atoms in condensate.

- Large number of atoms behaving coherently.

- Might be used to make an atom-laser.

Why simulate a BEC numerically?

- Analytic solutions make serious assumptions about the condensate.
- e.g. $T \approx 0$, or significantly below critical temperature.
- e.g. Mean-field theory.
- These assumptions are often not satisfied, particularily near critical temperature, or for small condensates.
- Analytic results do not always agree with experiment.
- Numerical simulations could make predictions in the regimes which do not satisfy the analytic assumptions.

Many-body problems

- if you have N bodies, each with D energy levels (say), then Hilbert space has

$$D^N$$

dimensions.

- e.g. for just 15 4-energy-level particles, that's about $(4^{15})^2$

$$\approx 1000\,000\,000\,000\,000\,000$$

simultaneous differential equations to solve.

- BEC's contain $10^3 - 10^9$ atoms!

- Exact solution of density matrix is impossible on a classical computer.

Stochastic equations to the rescue

- Using the *positive P distribution* we can reduce problem to $4\tilde{N}$ stochastic equations.

- $\tilde{N}$ is the number of momentum modes in the field. For a BEC, this is similar to number of atoms N.

- To calculate observeables, average over many realizations (trajectories).

- As number of trajectories grows, result approaches exact quantum mechanics.

- Very efficient — interesting quantities and main trends emerge from noise first.

- Used to simulate (e.g.) condensation of BEC. [Drummond & Corney, Phys. rev. A **60**, R2661 (1999)].

- There were 10,000 atoms, 32,000 momentum modes, $10^{10\ 000}$ states in Hilbert space!

- Problems after condensation: unmanageable noise.

- Solution (hopefully): improve P distribution.

Quantum model of a BEC

The usual non-relativistic Hamiltonian for neutral atoms in a trap $V(\mathbf{x})$, interacting via a potential $U(\mathbf{x})$, together with absorbing reservoirs $\widehat{R}(\mathbf{x})$, in $D = 2$ or $D = 3$ dimensions:

$$
\begin{aligned}
\widehat{H} &= \int d^D\mathbf{x}\left[\frac{\hbar^2 2m}{\nabla}\widehat{\Psi}^\dagger(\mathbf{x})\nabla\widehat{\Psi}(\mathbf{x})\right] \\
&+ \int d^D\mathbf{x}\left[V(\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x})\right] \\
&+ \int d^D\mathbf{x}\left[\widehat{\Psi}^\dagger(\mathbf{x})\widehat{R}(\mathbf{x}) + \widehat{\Psi}(\mathbf{x})\widehat{R}^\dagger(\mathbf{x})\right] \\
&+ \int\int d^D\mathbf{x}d^D\mathbf{y}\frac{U(\mathbf{x}-\mathbf{y})}{2}\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{y})\widehat{\Psi}(\mathbf{y})\widehat{\Psi}(\mathbf{x})\,.
\end{aligned}
$$

$\widehat{\Psi}(\mathbf{x})$ is the boson field at *spatial* position $\mathbf{x}$.

- Expand the boson field $\widehat{\Psi}(\mathbf{x})$ in momentum modes $\widehat{a}_{\vec{k}}$:

$$\widehat{\Psi}(\mathbf{x},t) = \sum_{\vec{k}} \left\{ \widehat{a}_{\vec{k}}(t)\ e^{i\vec{k}\cdot\mathbf{x}} \ + \ \widehat{a}^{\dagger}_{\vec{k}}(t)\ e^{-i\vec{k}.\mathbf{x}} \right\}$$

- The Hamiltonian now becomes

$$\widehat{H} \ = \ \hbar \sum_{i,j=1}^{m} \left[\omega_{ij}\widehat{a}_i^{\dagger}\widehat{a}_j + \frac{\chi_{ij}}{2}\widehat{n}_i\widehat{n}_j \right]$$

+ trap potential and damping terms
also include reservoir in
master equation

where: $\widehat{n}_i = \widehat{a}_i^{\dagger}\widehat{a}_i$

- The $\widehat{n}_i\widehat{n}_j$ terms are the most important.

Positive P distribution?

- Expand density matrix $\widehat{\rho}$ as a weighted sum of coherent state elements $||\vec{\alpha}>$:

$$\widehat{\rho} = \int \; P(\vec{\alpha}, \vec{\beta}) \; \frac{||\vec{\alpha}><\vec{\beta}||}{<\vec{\beta}||\vec{\alpha}>} \; d^{2\tilde{N}}\vec{\alpha} \; d^{2\tilde{N}}\vec{\beta}$$

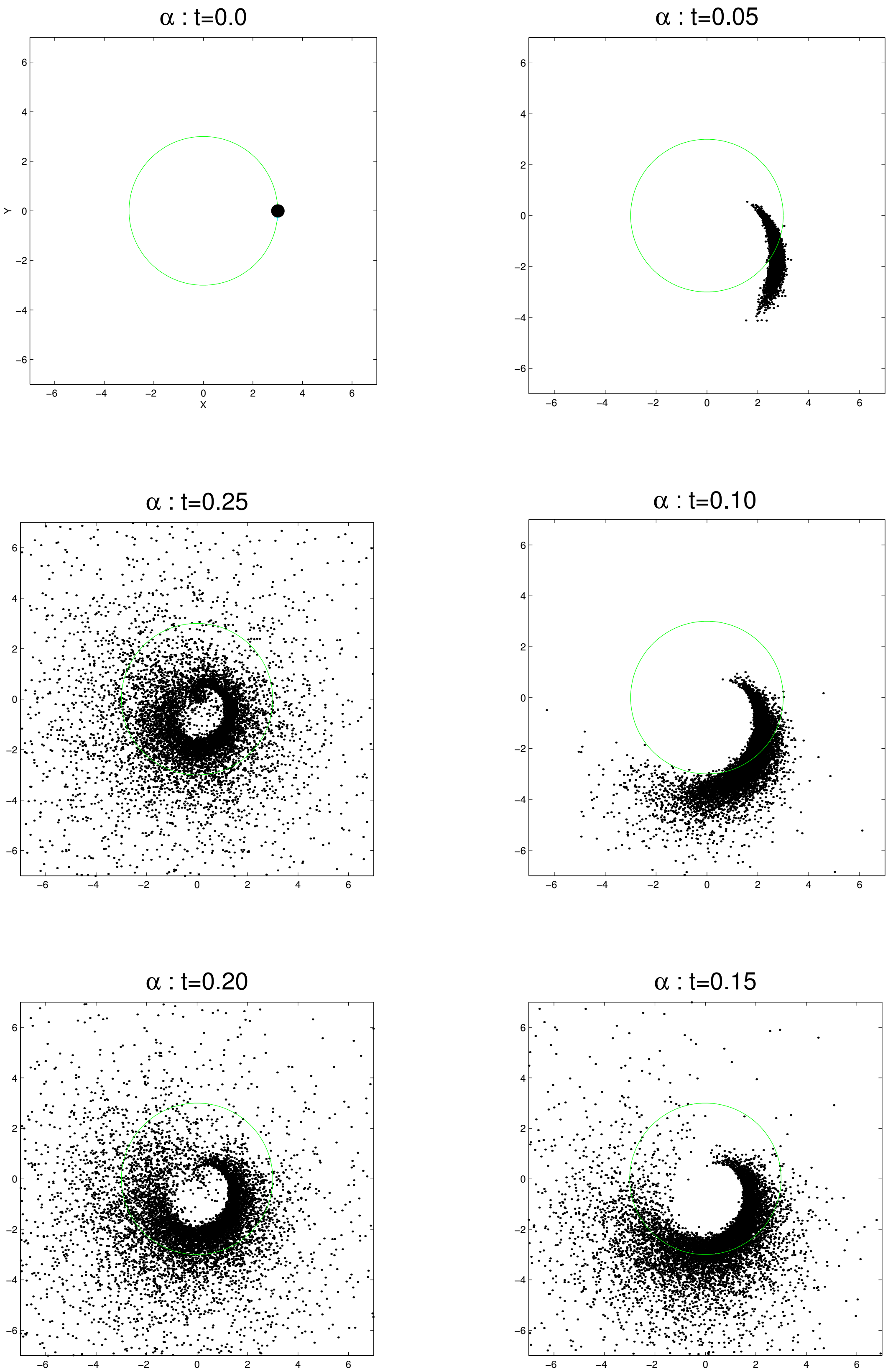
- Where $\vec{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_i, \ldots, \alpha_{\tilde{N}}]$,

- and

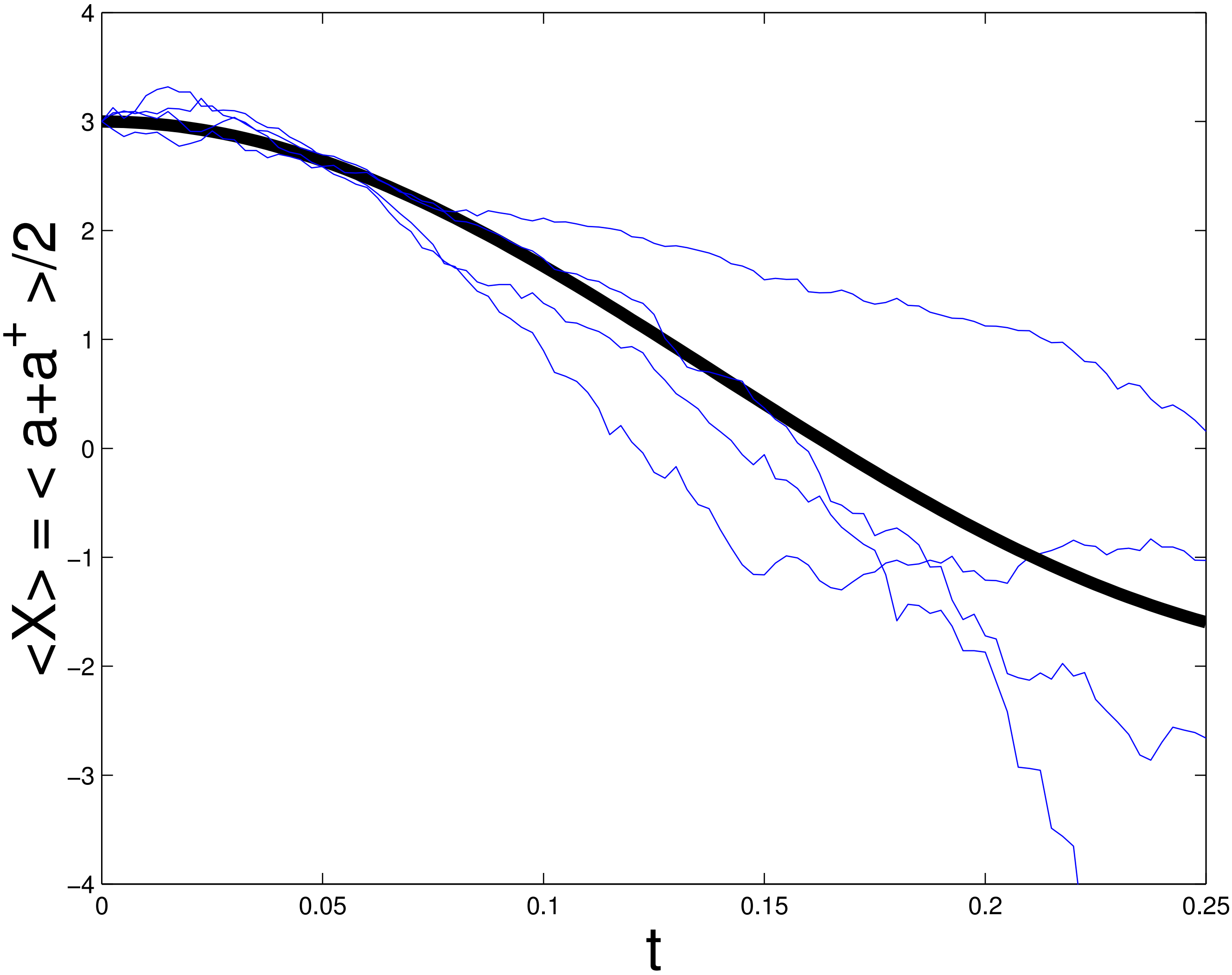
$$||\vec{\alpha}>= e^{\sum_i \alpha_i \widehat{a}_i^\dagger}|0>$$

  is un-normalised.

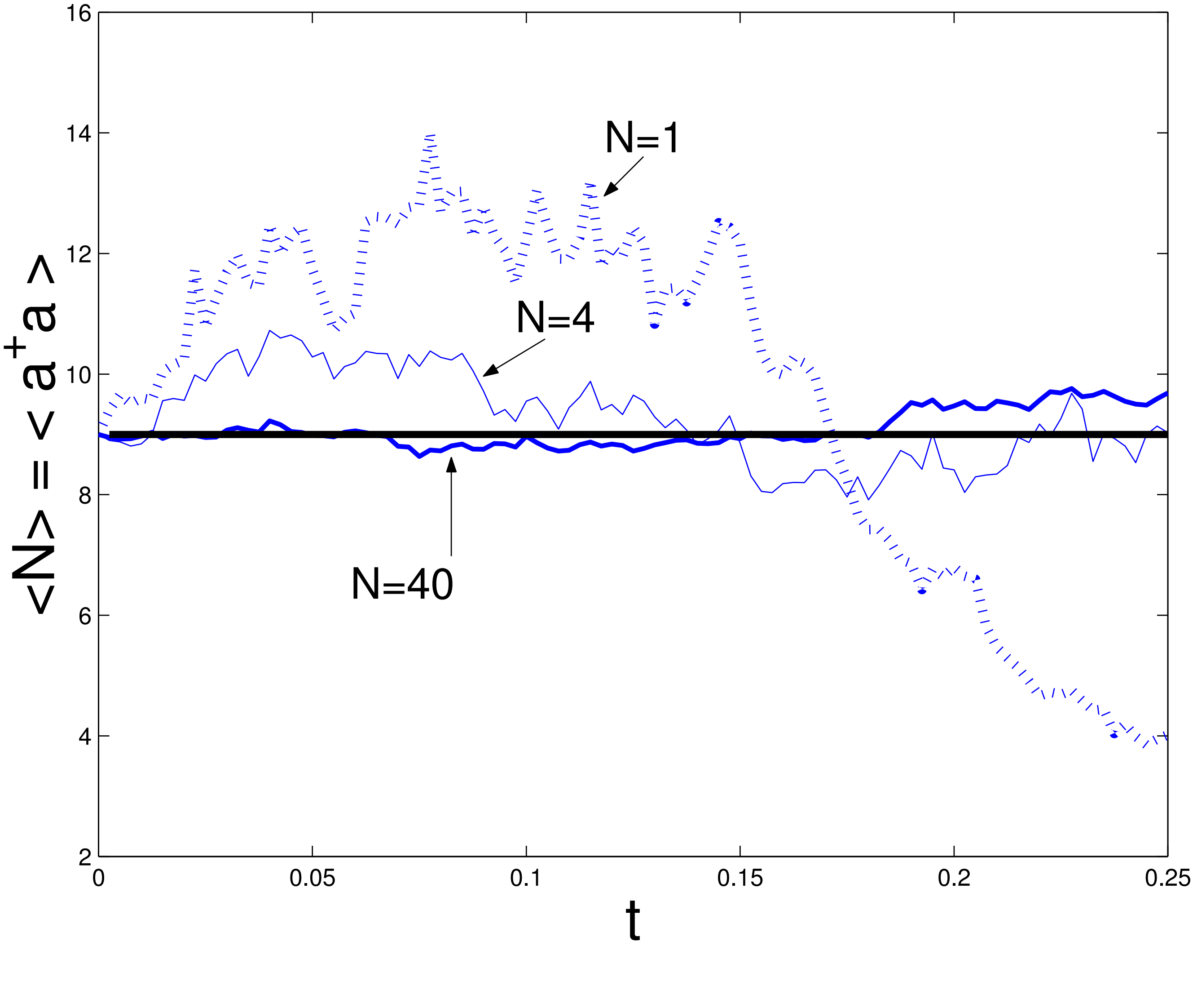
- $\widehat{a}_i^\dagger$ is the creation operator for the ith momentum mode of the field. (Like in quantum optics)


α : t=0.0
Y
X
α : t=0.05
α : t=0.25
α : t=0.10
α : t=0.20
α : t=0.15

Individual paths, and the mean:



Averages over different numbers of paths:



Important toy problem

- The noise problem in BEC simulations is due to the $\chi_{ij}(\hat{a}_i^\dagger \hat{a}_i)(\hat{a}_j^\dagger \hat{a}_j)$ terms in the hamiltonian.

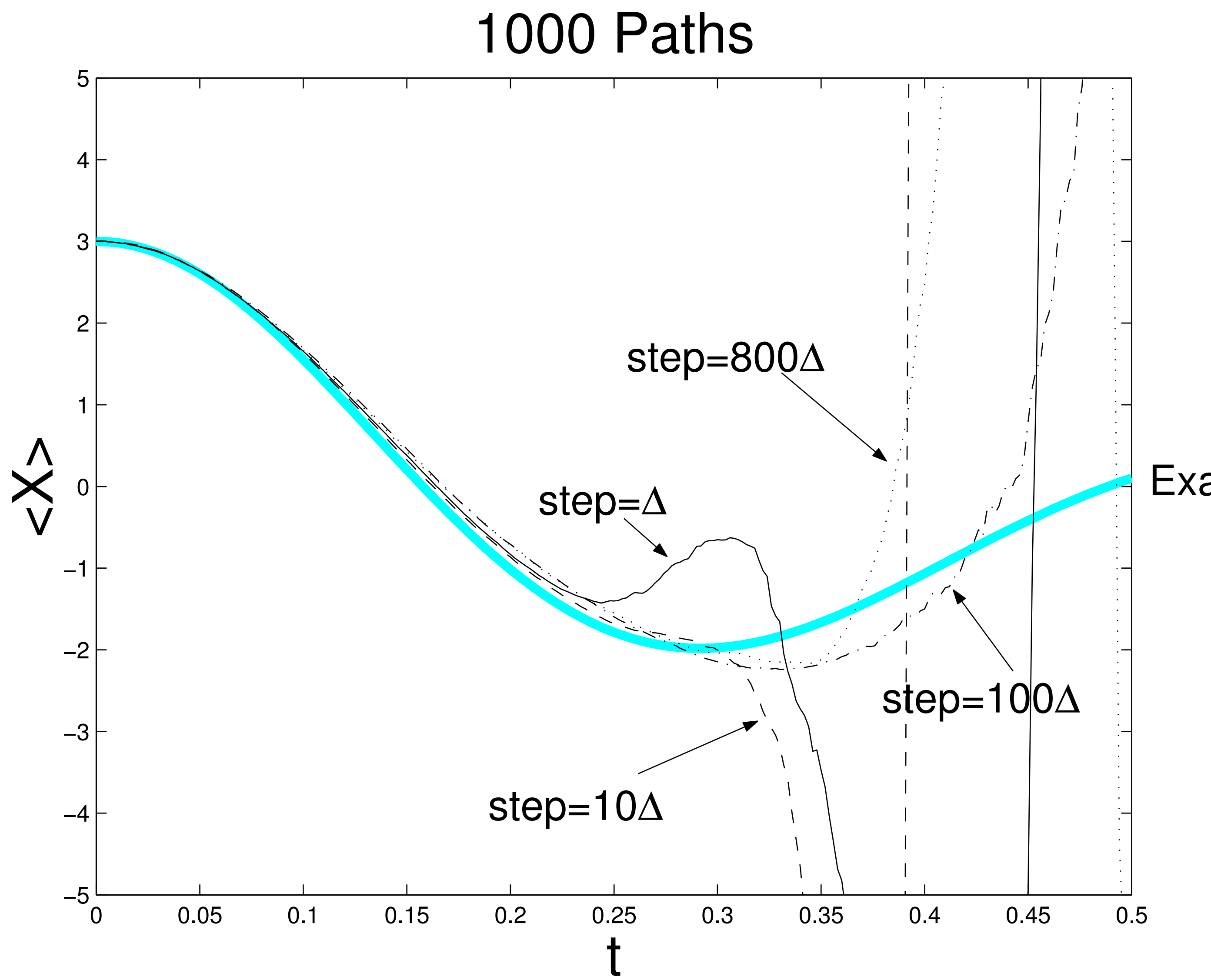
- The one-mode *anharmonic oscillator*, a very simplified BEC hamiltonian shows the same noise problems:

$$\hat{H} = \frac{\chi}{2}(\hat{a}^\dagger \hat{a})^2$$

- If we could fix the noise problem for this toy system, we should be able to fix it for the full BEC.

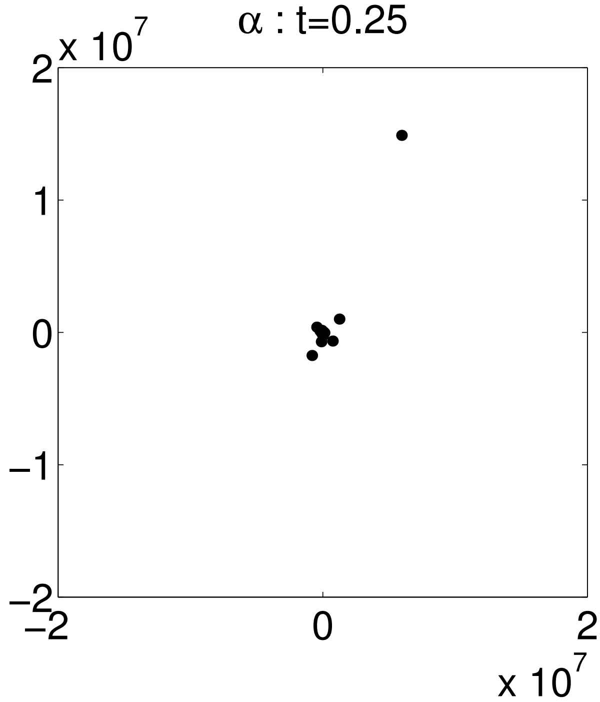
Intractable noise

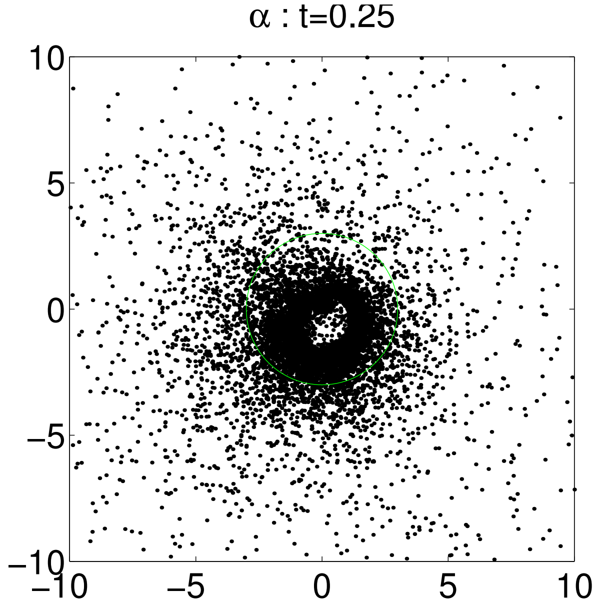
consider the 1D case $H = \hbar(\hat{a}^\dagger \hat{a})^2$



The positive P-distribution does well up to a certain time, but unfortunately after about $t \approx 0.3$, the $< X >$ errors are resistant to step size.

What is the problem?





Hermitian P distribution?

$$\widehat{\rho} = \int \ P(\vec{\alpha}, \vec{\beta}, \theta) \ \frac{\widehat{\Lambda}}{\mathrm{Tr}[\widehat{\Lambda}]} \ d^{2\tilde{N}}\vec{\alpha} \ d^{2\tilde{N}}\vec{\beta} \ d\theta$$

$$\widehat{\Lambda} = e^{i\theta} || \vec{\alpha} >< \vec{\beta} || + e^{-i\theta} || \vec{\beta} >< \vec{\alpha} ||$$

New identities:

$$\left(i \frac{\partial^2}{\partial\alpha\partial\theta} \ + \ \frac{\partial}{\partial\alpha} \right) \widehat{\Lambda} \qquad = \qquad 0$$

$$\left(i \frac{\partial^2}{\partial\beta\partial\theta} \ + \ \frac{\partial}{\partial\beta} \right) \widehat{\Lambda} \qquad = \qquad 0$$

$$\left(\frac{\partial^2}{\partial\theta^2} \ + \ 1 \right) \widehat{\Lambda} \qquad = \qquad 0$$

Equations with stochastic gauges G,$\bar{G}$.

$$
\begin{aligned}
d\alpha &= -i\alpha[\ \{\alpha\beta^* + \frac{1}{2} \\
&\quad - G(1+i)(T+i)\}dt \ + \ \sqrt{i}\, dW\ ] \\
d\beta &= -i\beta[\ \{\alpha^*\beta + \frac{1}{2} \\
&\quad - \bar{G}(1-i)(T+i)\}dt \ + \ \sqrt{i}\, d\overline{W}\ ] \\
d\tilde{\theta} &= -2T(G^2 + \bar{G}^2)dt \ + \ \sqrt{2}\,[GdW + \bar{G}d\overline{W}]
\end{aligned}
$$

with

$$
\begin{aligned}
\tilde{\theta} &= \theta + \mathrm{Im}[\alpha\beta^*] \\
T &= \tan(\tilde{\theta})
\end{aligned}
$$

The noises dW and $d\bar{W}$ are random, Gaussian, mutually uncorrelated, and uncorrelated for different times, with variance

$$< dW(t)dW(t) >= dt$$

When the gauges G and $\bar{G}$ are zero the equations are identical to those obtained using the positive P-distribution.

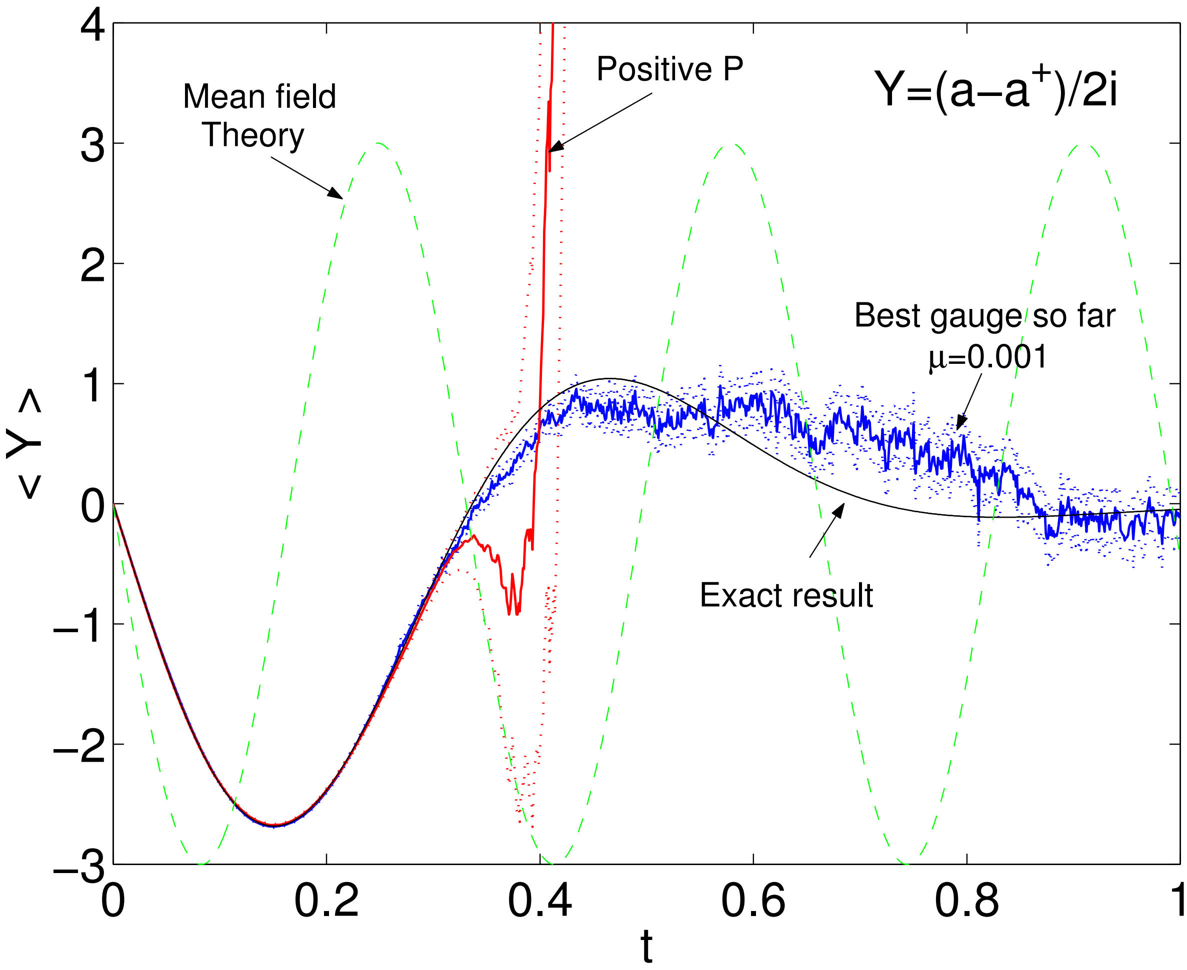
Stochastic Gauges

- The functions G are arbitrary. A good choice turns out to be
$$\begin{aligned} G &= \frac{\mu}{2}\Big(|\alpha|^2 - \mathrm{Re}[\alpha\beta^*(1+i)]\Big) \\ \bar{G} &= \frac{\mu}{2}\Big(|\beta|^2 + \mathrm{Re}[\alpha\beta^*(1-i)]\Big) \end{aligned}$$
with a free parameter μ deciding how much the new equations vary from the old positive P version.

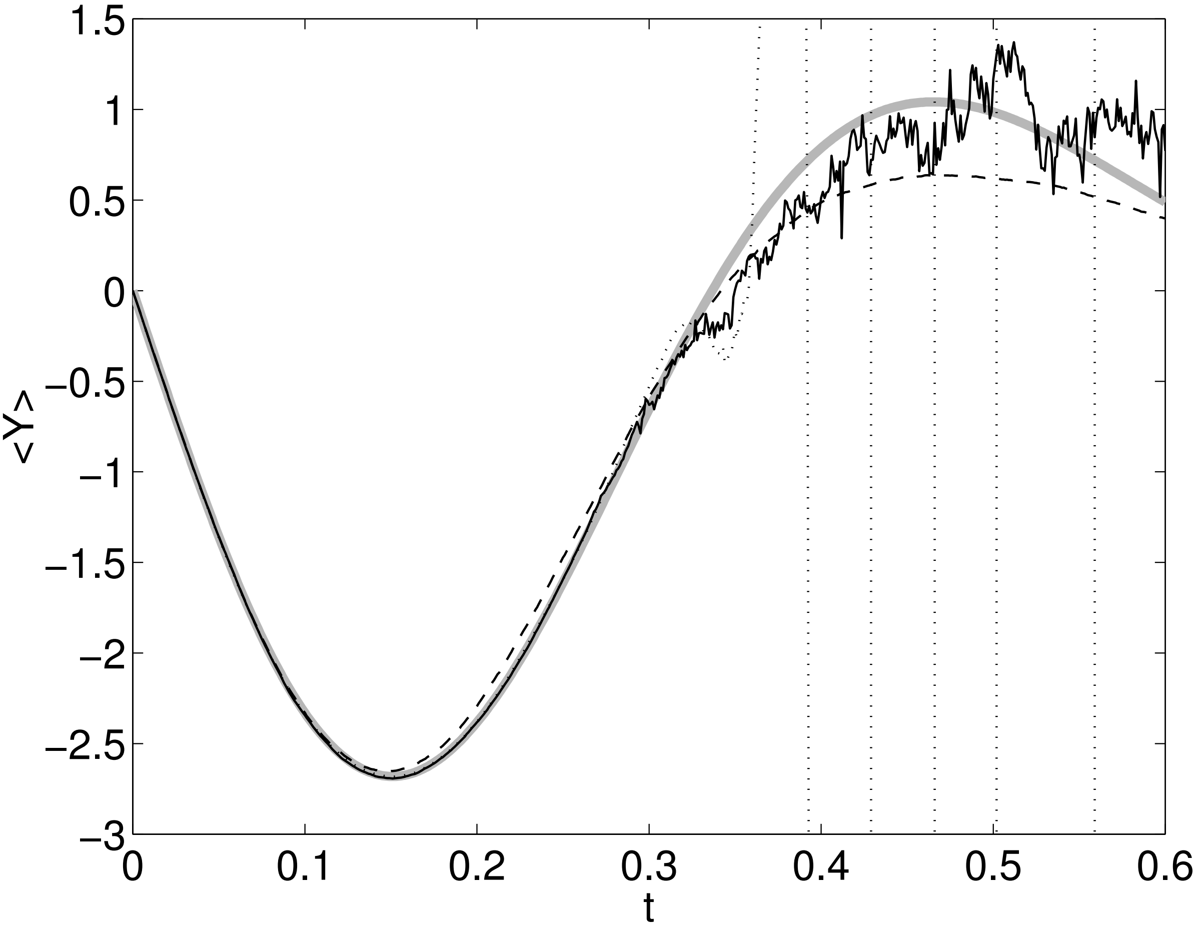
- This gauge contains all α,β trajectories within a finite radius from zero in phase-space.

- Tradeoff: This radius is small for large μ, but non-zero boundary terms spoil the calculation due to systematic errors. For μ small, the systematic errors are negligible, but the noise is larger.

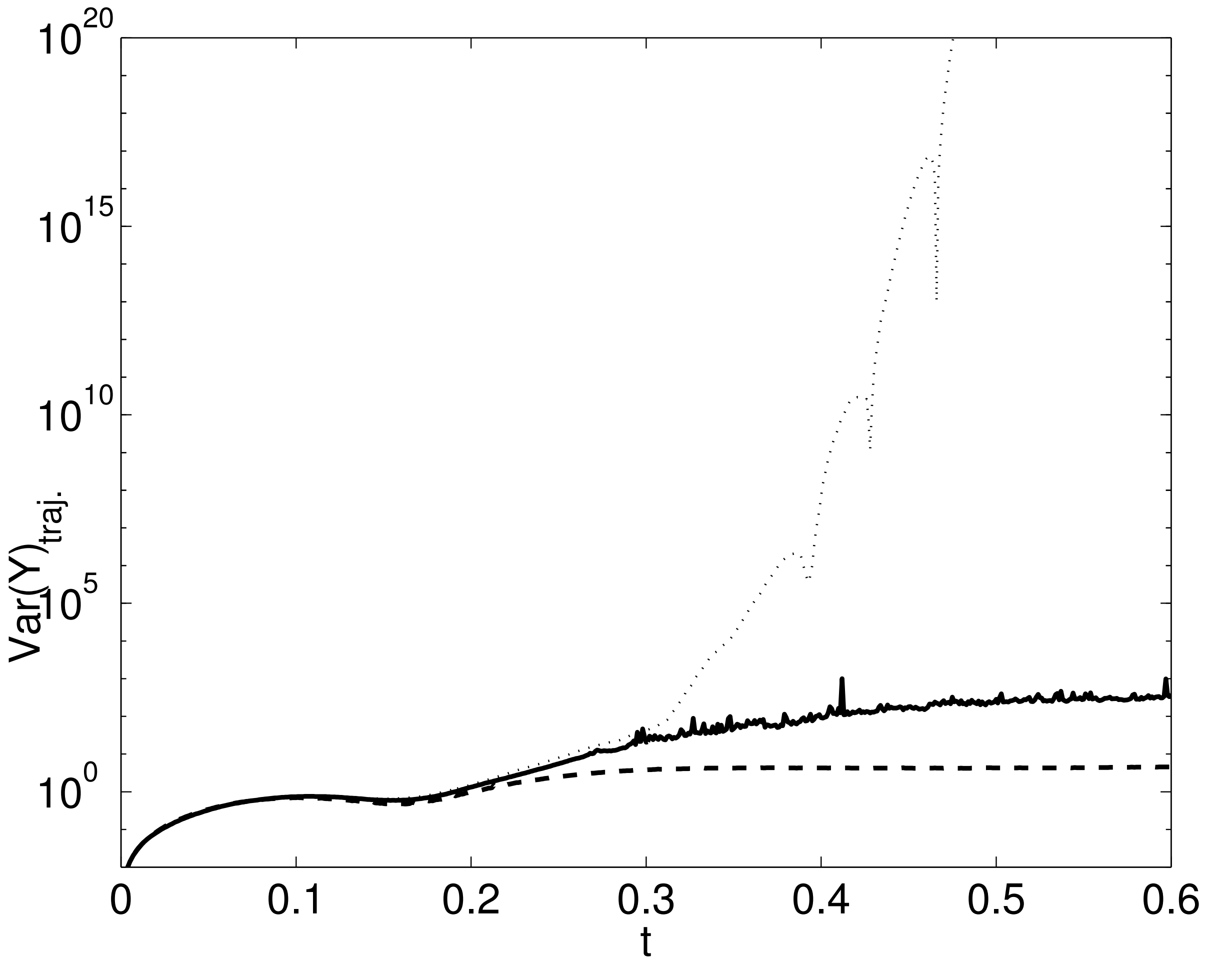
- $\mu = 0.001$ is a good choice.



Comparison of simulations of the quadrature $\hat{Y} = \frac{1}{2i}(\hat{a} - \hat{a}^\dagger)$ for an initial coherent state $\mid 3 >$ acted on by $\hat{H} = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a})^2$. $10,000$ trajectories.



Comparison of simulations of the quadrature $\hat{Y} = \frac{1}{2i}(\hat{a} - \hat{a}^{\dagger})$ for an initial coherent state $|\ 3 >$ acted on by $\hat{H} = \frac{\hbar}{2}(\hat{a}^{\dagger}\hat{a})^2$. 10,000 trajectories. Thick shaded line: exact result; Dotted line: Positive P distribution; Dashed line: $\mu = 1$ Hermitian gauge — note the systematic error!; Solid line: $\mu = 0.001$ Hermitian gauge.



Comparison of sampling errors for various stochastic simulations: "old" positive P ($\mu = 0$), small sampling hermitian P ($\mu = 1$), best hermitian P ($\mu = 0.001$). Shown is the variance in quadrature $\hat{Y}$. Size of actual sampling uncertainty in calculated moment for N trajectories is $\sqrt{\mathrm{Var}(\hat{Y})/N}$, hence number of trajectories needed for an a accurate result grows as $\mathrm{Var}(Y)$. Note the logarithmic scale!

Some Conclusions

- For $(\hat{n})^2$ anharmonic interactions, sampling error is reduced by many orders of magnitude, allowing numerical simulations of systems for which these are important.

- Bose-Einstein Condensates are such systems.

- The computational overheads (number of equations) for Positive-P type methods scale *linearly* with number of subsystems!

- When the last "kinks" are ironed out of this method, it should be possible to perform full quantum simulations of BEC's.

- During our investigations into appropriate gauges, we have observed that the optimal choice of gauge may depend on which observable one is interested in. Taking this into account may lead to further improvement in calculation efficiency.

- The stochastic gauge approach could be used to improve quantum simulations of many systems, also with other quasi-probability distributions.

Thank You