Simulating Quantum Evolution of Many-Many Body Systems

(And particularily, Bose-Einstein Condensates)

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(Work in progress with P. Drummond)

Many-Many Body Problems

It has been (and is) claimed (e.g. famously by Feynman) that full quantum evolution of systems involving a large number of bodies is impossible to model on classical computers.

The idea being that if you have N bodies, each with D energy levels (say), then Hilbert space has

$$D^N$$

dimensions.

e.g. for just 20 10-energy-level particles, that's

$$100,000,000,000,000,000,000$$

simultaneous differential equations to solve.

(piece of cake!)

But. . .

BEC's

The Hamiltonian for a N particle BEC contains terms of the sort

$$\hat{a}_i^\dagger \hat{a}_j$$

absorption terms

$$\boxed{\hat{a}_i^{\dagger 2} \hat{a}_j^2}$$

Where the $\hat{a}_i$ are anihilation operators for field modes i.

The number of significant modes is again of the order of N.

But now, rather than solving for each element in the density matrix, let's do something more cunning...

Positive P distribution

Since the full quantum state $\widehat{\rho}(t)$ may be complicated, let's try writing it as a weighted combination of simpler states. How about **coherent** states?

It is much easier to solve for the behaviour of a coherent state under our Hamiltonian, and then we'll add up the solutions according to their weights, and find how the more complicated state has evolved.

Better still: It is even easier to find out how a coherent state $|\alpha>$ changes over an infinitesimal time dt. Then we can write a differential equation, and let a computer do the hard work!

For now, consider a single mode.

Let us write the state of the full system as

$$\begin{aligned} \widehat{\rho} &= \sum_{\text{all } \alpha \ \& \ \beta} P(\alpha,\beta)|\alpha><\beta| \\ &\to \int P|\alpha><\beta| \ d^2\alpha \ d^2\beta \end{aligned}$$

If we consider a single element $|\alpha><\beta|$, after time dt it will become a weighted sum of the nearby elements. So in the end we get a differential equation for $P(\alpha,\beta)$.

Typically we might have

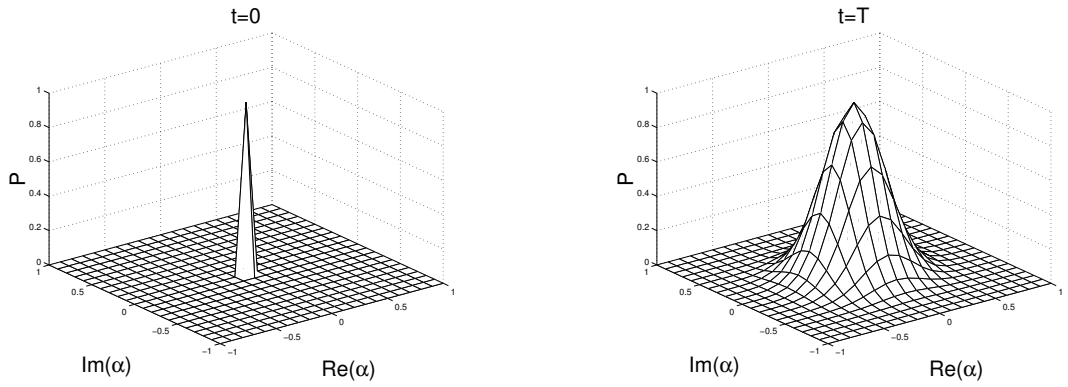
$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial \alpha}(AP) + \frac{\partial^2}{\partial \alpha^2}(DP) + \ \partial\beta \text{ terms}$$

For N modes , P will be a function of $2N$ complex variables ($4N$ real variables).

Now for a trick!

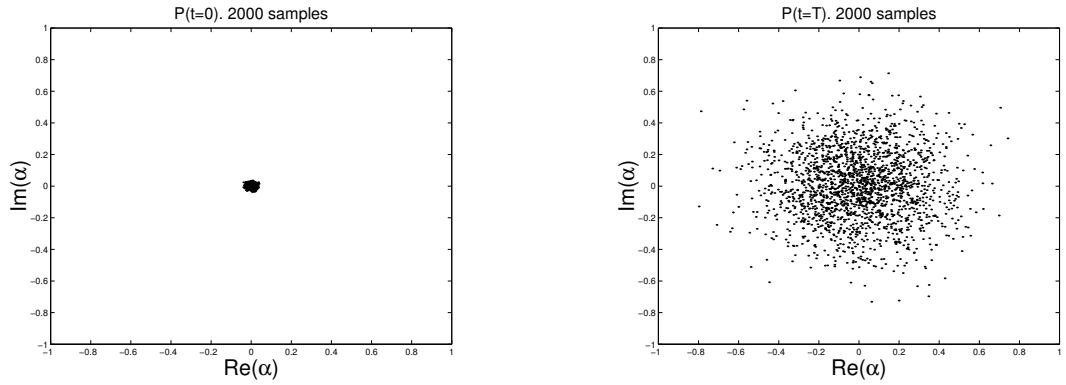
Suppose we have a coherent state initially, and it evolves to a Gaussian. This would correspond to

$$\frac{\partial P}{\partial t} = \frac{\partial^2}{\partial \alpha^2} P$$



This is like random diffusion, or Brownian motion. which can be modeled with gaussian noise of variance dt:

$$d\alpha = \sqrt{2} dW$$



We can do this for more complicated differ-

The beauty of this is that now if we have N modes, we only have $2N$ *first order* (complex) differential equations (with noise).

Compare this to the D^N needed with the head-on matrix element approach!

To get the expectation value of an observeable, we calculate some large number of random trajectories, and average an appropriate function over them.

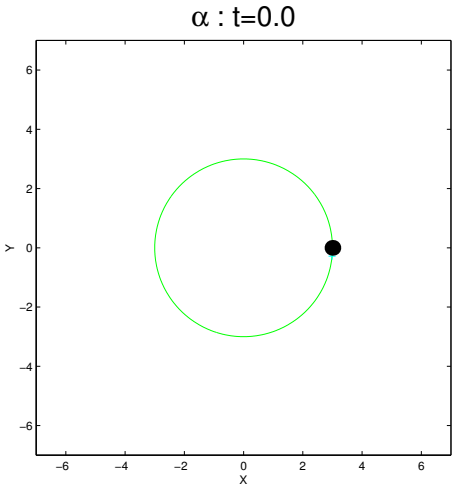
For example the photon number,

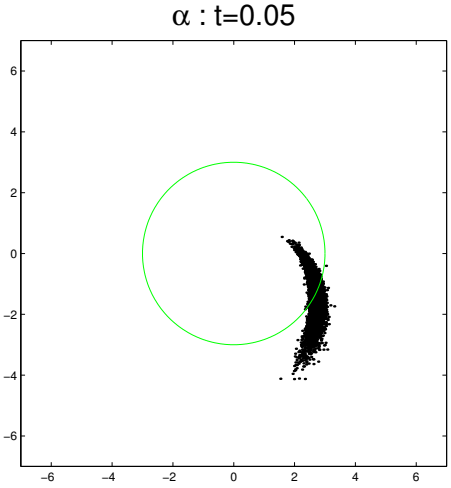
$$E(\hat{a}^\dagger \hat{a})$$

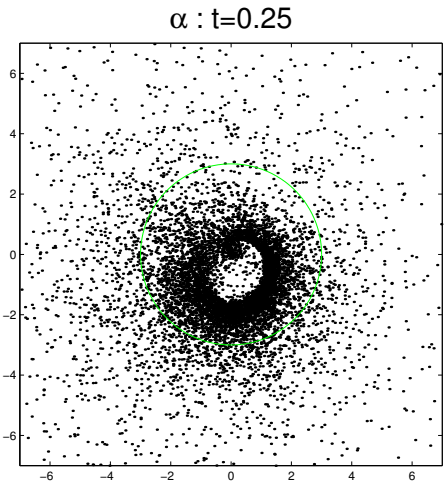
is given by the average over all randomly generated trajectories

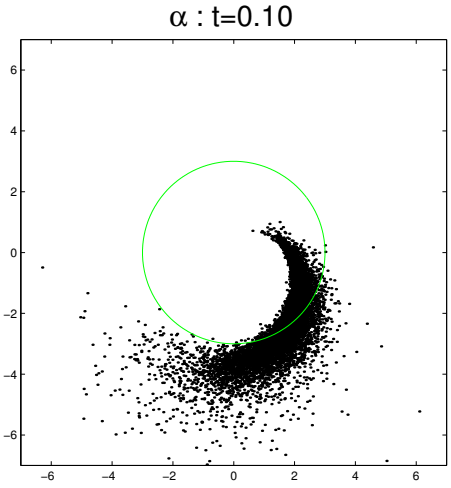
$$< \alpha\beta^* >$$

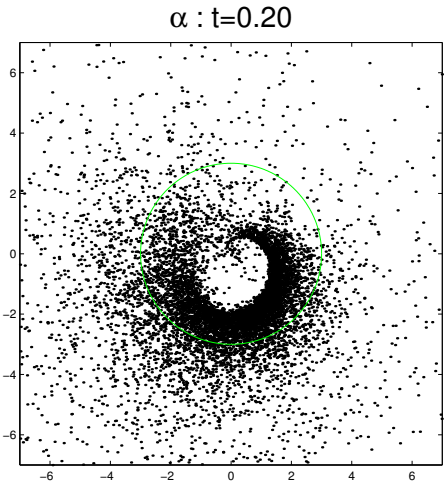
Time for some pictures!

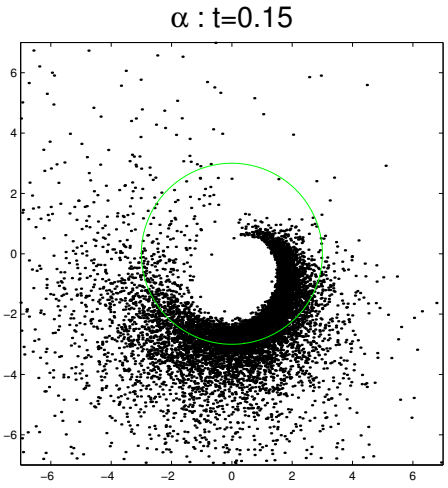

α : t=0.0
Y
X


α : t=0.05

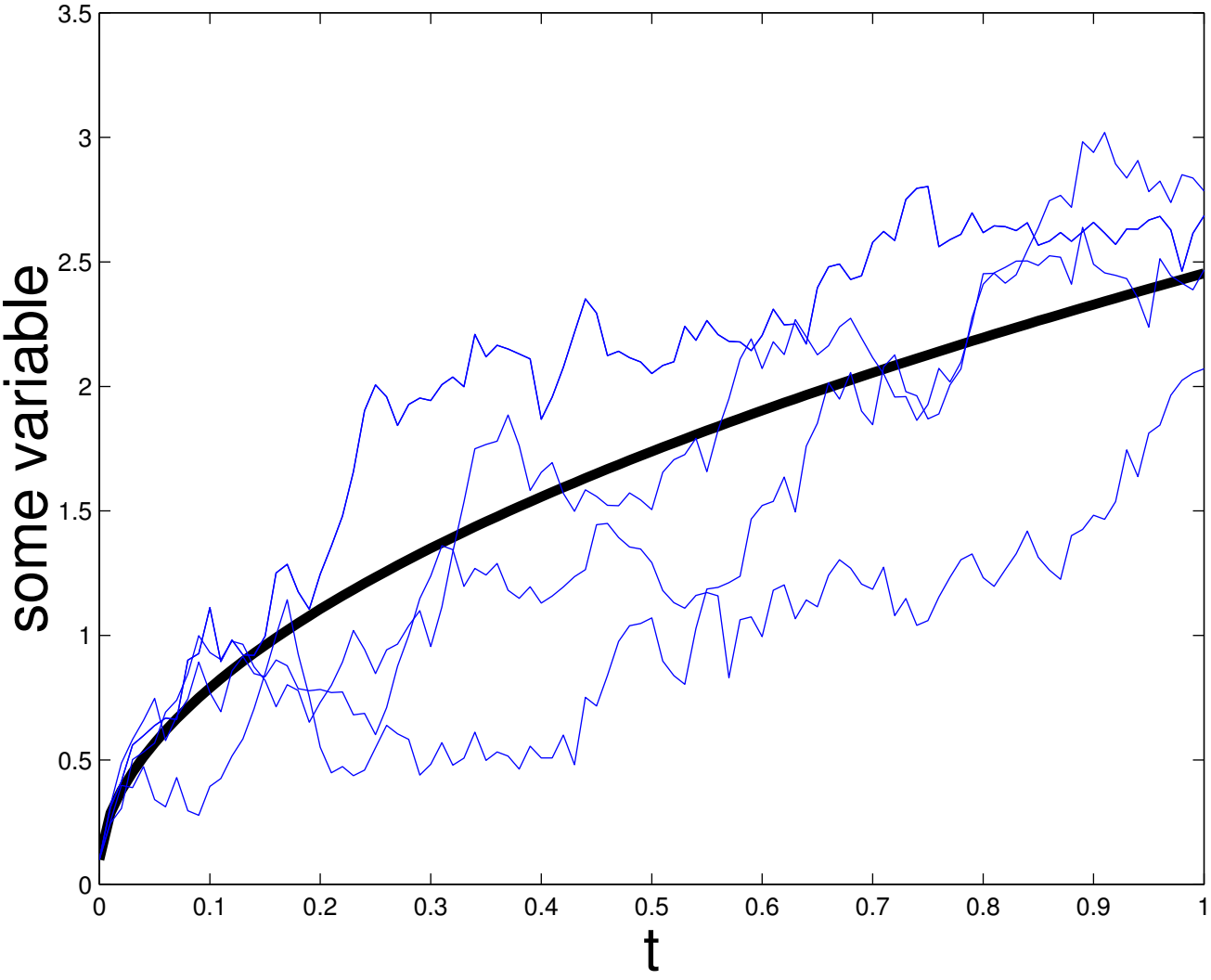

α : t=0.25


α : t=0.10

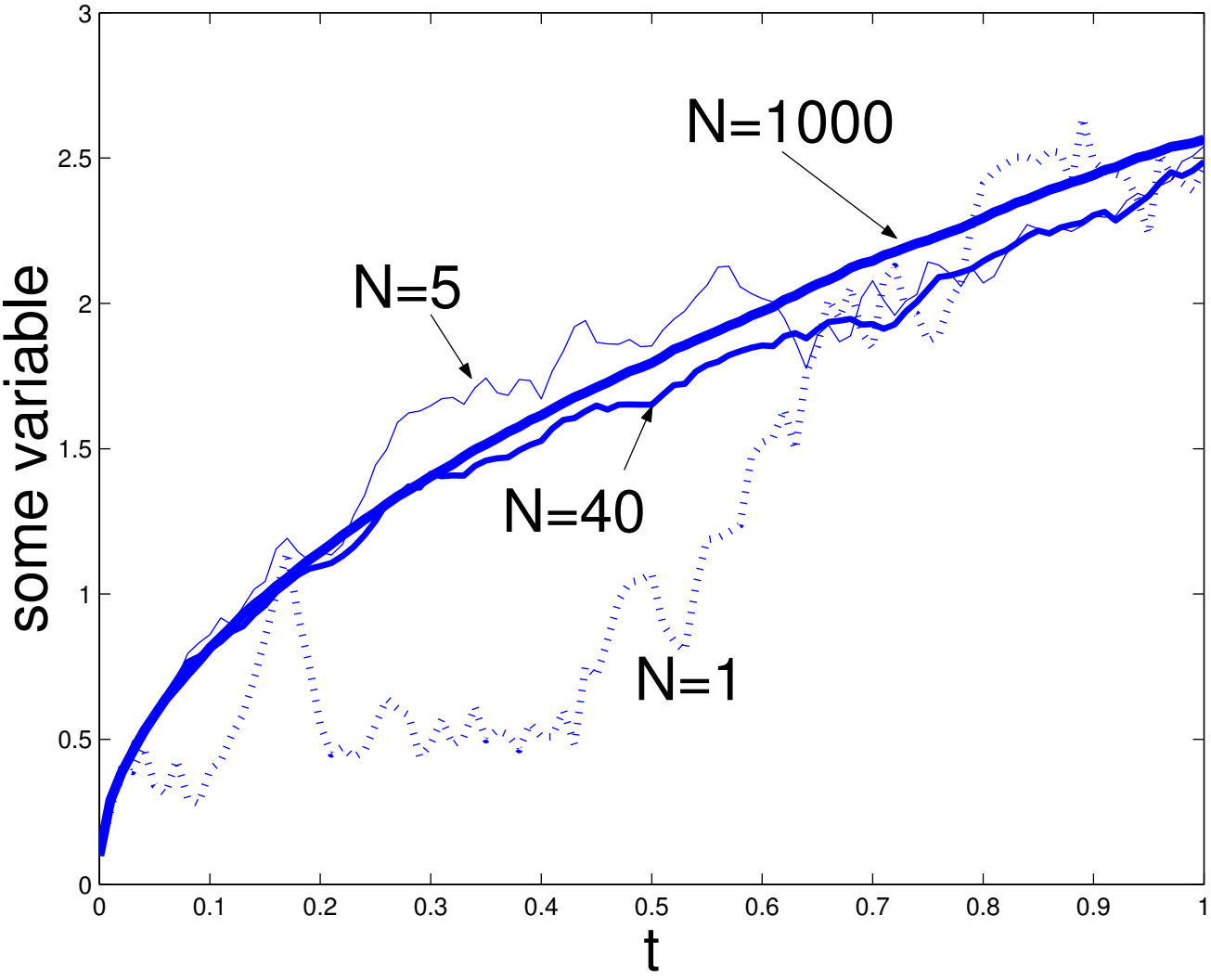

α : t=0.20

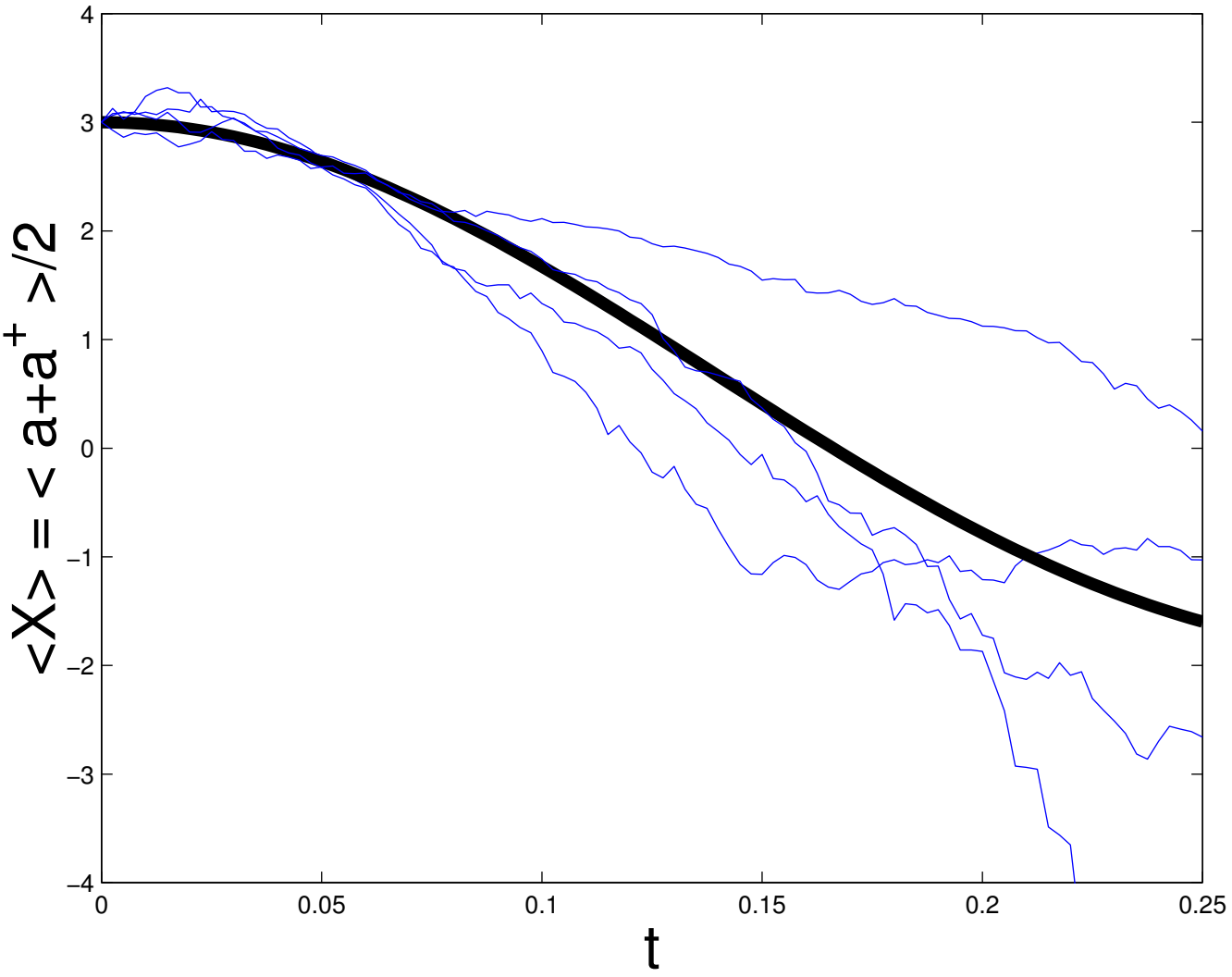

α : t=0.15

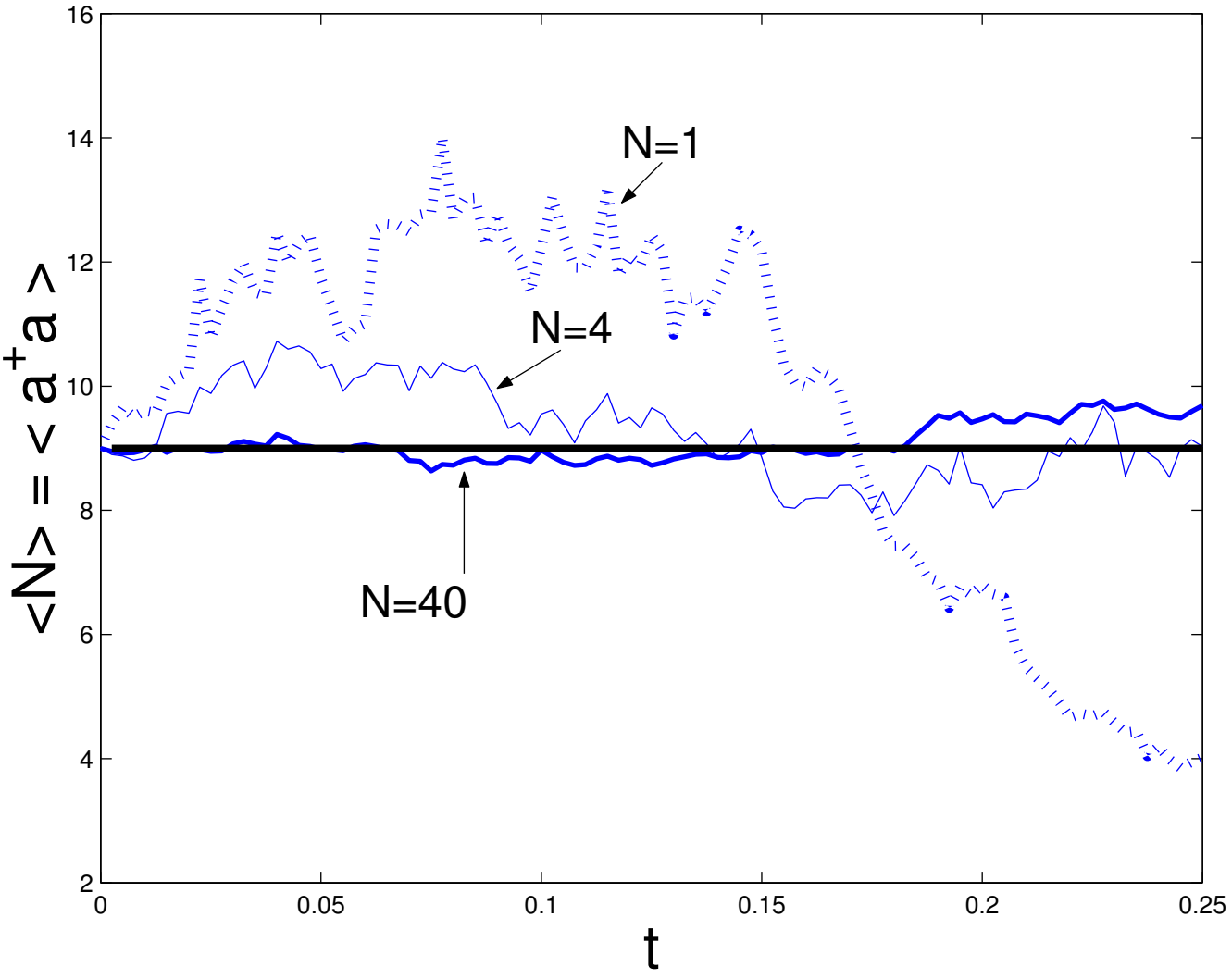
Individual paths, and the mean:



Averages over different numbers of paths:




4
3
2
1
0
−1
−2
−3
−4
0
0.05
0.1
0.15
0.2
0.25
t
<X> = < a+a+ >/2


16
14
12
10
8
6
4
2
0
0.05
0.1
0.15
0.2
0.25
t
<N> = < a+ a >
N=1
N=4
N=40

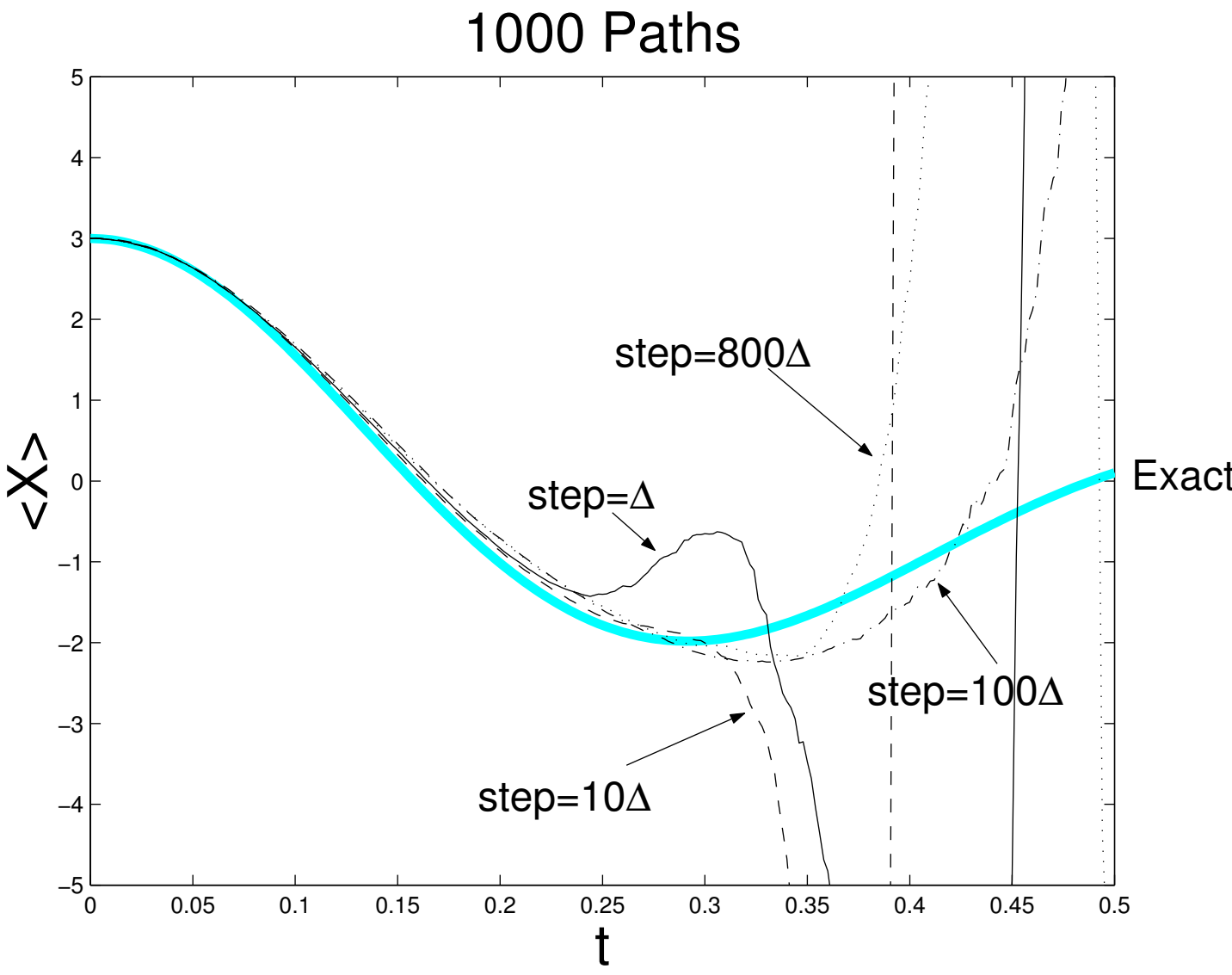
E.g: Drummond and Corney successfully treated the evaporative cooling of ions, and formation of a BEC using the positive P-distribution.

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

There were 10,000 atoms!

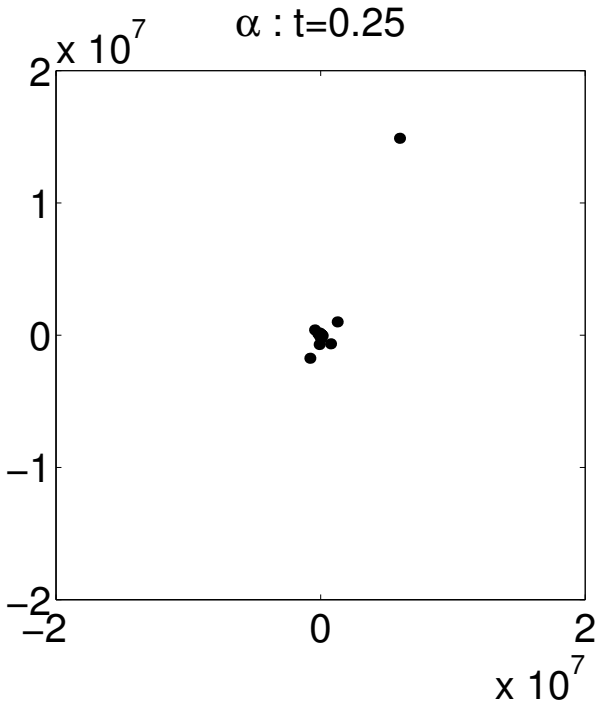
a problem:

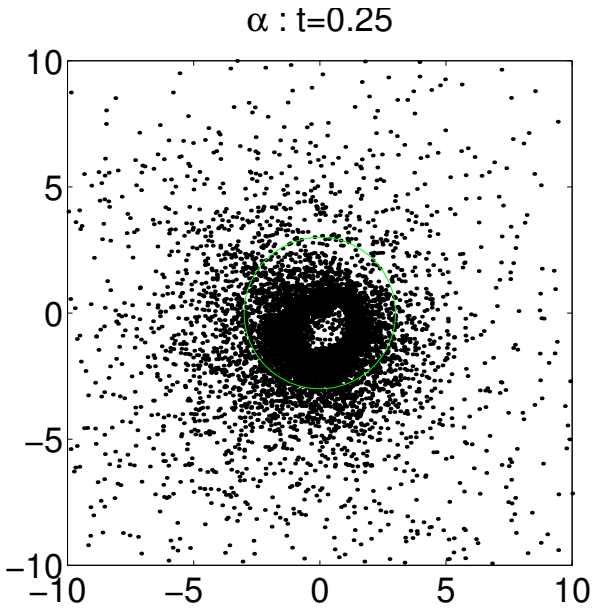
consider the 1D case $H = \hbar(\hat{a}^\dagger \hat{a})^2$



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.

Why? Long tails on the distribution.





Recently we have been trying a different expansion, with very promising results.

$$\hat{\rho} \;=\; \sum_{\text{all } \alpha \;\&\; \beta} P(\alpha,\beta)\left[e^{i\theta}|\alpha><\beta| + e^{-i\theta}|\beta><\alpha|\right]$$

Here the "basic states" are Hermitean. This makes them more like real quantum states than the $|\alpha><\beta|$ that were used previously.

This gives more complicated equations, but we can let the computer slave away at them.

previous equations...

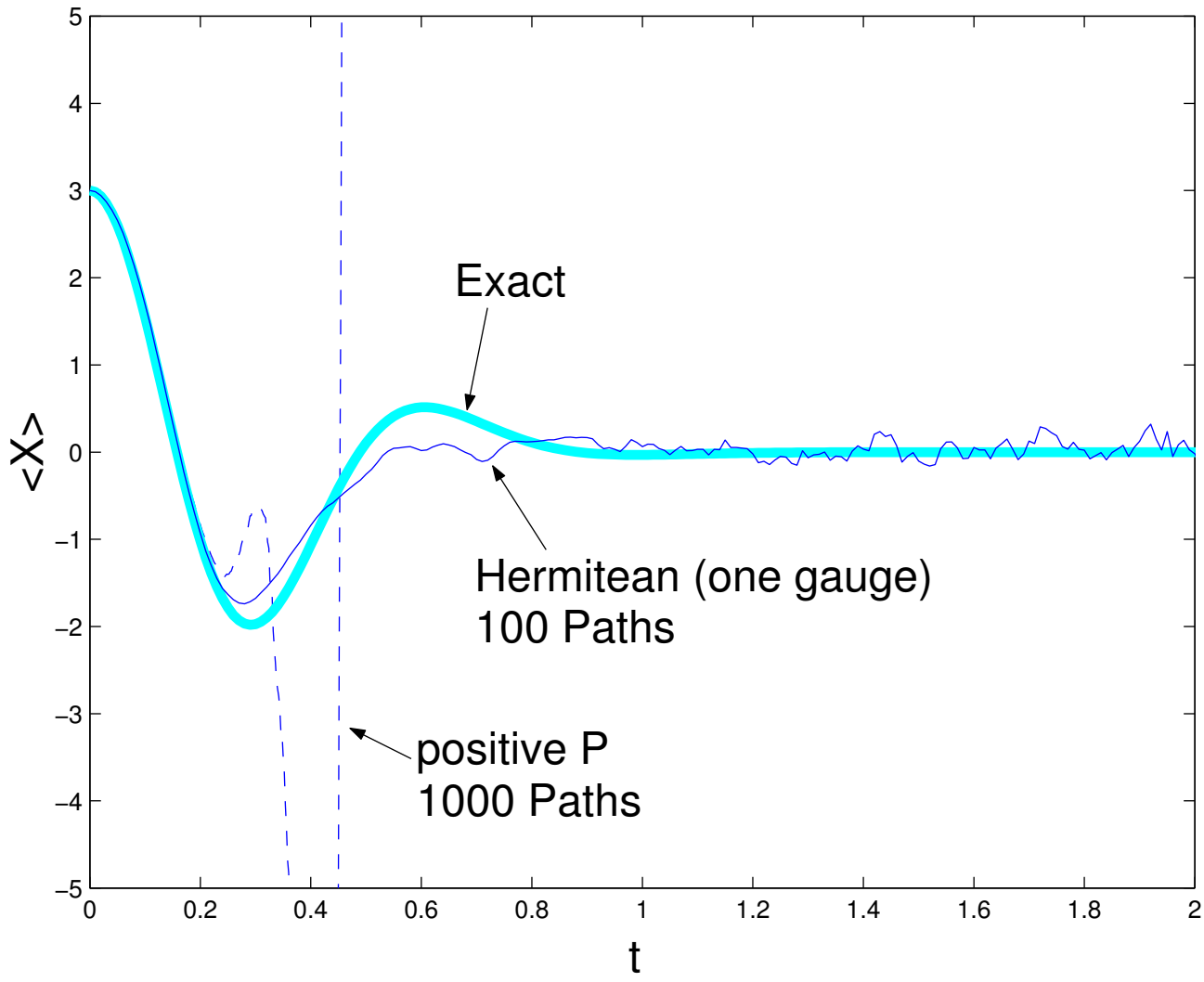
$$\begin{aligned}\dot{\alpha} &= -i\alpha(1/2 + \bar{\alpha}\alpha) + (1-i)\alpha/\sqrt{2}\xi \\ \dot{\bar{\alpha}} &= i\bar{\alpha}(1/2 + \bar{\alpha}\alpha) + (1+i)\bar{\alpha}/\sqrt{2}\bar{\xi}\end{aligned}$$

New equations...

$$
\begin{aligned}
\dot{x} &= \frac{1}{2}\left[(n_1+n_2)+T(n_1-n_2)+2FT\right]+\xi \\
\dot{\bar{x}} &= \frac{1}{2}\left[(n_1-n_2-T(n_1+n_2)-2\bar{F}T\right]+\bar{\xi} \\
\dot{y} &= F \\
\dot{\bar{y}} &= \bar{F} \\
\dot{\theta} &= -F\left\{\frac{1}{2}\left[n_1+n_2+T(n_1-n_2)+2TF\right]+F\xi\right\} \\
&\quad +\bar{F}\left\{\frac{1}{2}\left[n_1-n_2-T(n_1+n_2)-2T\bar{F}\right]+\bar{F}\bar{\xi}\right\}
\end{aligned}
$$

where

$$
\begin{aligned}
n_1 &= \exp\left[(x+\bar{x}+y+\bar{y})/2\right]\cos\left[(y-\bar{y}-x+\bar{x})/2\right] \\
n_2 &= \exp\left[(x+\bar{x}+y+\bar{y})/2\right]\sin\left[(y-\bar{y}-x+\bar{x})/2\right] \\
T &= \tan(\theta+n_2) \\
F &= -|\alpha|^2/2 \\
\bar{F} &= -|\beta|^2 \\
\alpha &= exp\left[(1-i)(x+iy)/2\right] \\
\beta &= exp\left[(1-i)(\bar{x}+i\bar{y})/2\right]
\end{aligned}
$$


Exact
Hermitean (one gauge)
100 Paths
positive P
1000 Paths
<X>
t
5
4
3
2
1
0
−1
−2
−3
−4
−5
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Comments:

- The ultimate aim is to simulate a BEC, but we have only done the 1D case in this new expansion so far.

- This is because of the small discrepancy between numerical and analytical results which we want to fix! We now believe it is probably due to the stiffness of the equations.

- Varying the positive P approach in such ways may give computational improvements for many quantum systems.

Thank You