Simulating the quantum dynamics of a BEC

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Outline

- Why are first principles many-body calculations hard?

- How the positive P-distribution can simulate the formation of a BEC

- Unfortunately, it can't simulate a BEC's evolution due to quartic terms in the Hamiltonian.

- How this problem has been overcome for a single momentum-mode quartic hamiltonian, (which displays the same problemetic numerical behaviour), by using a new Hermitian P-distribution.

- This should be able to lead to a full simulation of a BEC's evolution.

Some quotes:

- "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*)

- "The equivalent to Molecular Dynamics . . . does not exist in any practical sense . . . One is forced to either simulate very small systems (i.e. less than five particles) or to make serious approximations." (David M. Ceperley, *Lectures on Quantum Monte Carlo*, May 1996)

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. . .

But. . . you can simulate the state evolution usingphase-space methods, which lead to stochastic equations. In many cases you only have

$$\text{some constant} \quad \times \quad N$$

stochastic equations!

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

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

There were 10,000 atoms!

Clearly stochastic methods are useful here!

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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 $\hat{R}(\mathbf{x})$, in $D = 2$ or $D = 3$ dimensions:

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

Momentum mode model

- Expand the field $\hat{\Psi}(\mathbf{x})$ using free-field modes, with a maximum momentum cutoff $|k|_{\text{max}}$.

- Provided $|k|_{\text{max}} \ll a_0^{-1}$, where a_0 is the S-wave scattering length, $U(\mathbf{x}-\mathbf{y})$ can be replaced by a delta function.

With anihilation operators $\hat{a}_i$ for the ith mode, we can write

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

+ trap potential and damping terms

also include reservoir in master equation

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

- The condensation of a BEC has been simulated with Positive P distribution methods on the lattice model above, but sampling error destroys the simulation after the time of condensation.

- The positive P method works well for the $\hat{a}_i^\dagger \hat{a}_j$ and damping terms, but cannot handle terms like $(\hat{a}^\dagger \hat{a})^2$ for longer times.

- Need a method with much less sampling error for the $(\hat{a}^\dagger \hat{a})^2$ Hamiltonian.

- Have found one. See below!

Positive P representation

A quick review

$$\widehat{\rho} = \int P(\boldsymbol{\alpha},\ \boldsymbol{\beta})\ \frac{|\ \boldsymbol{\alpha}><\boldsymbol{\beta}\ |}{<\boldsymbol{\beta}\ |\ \boldsymbol{\alpha}>}\ d^{2n}\boldsymbol{\alpha}\ d^{2n}\boldsymbol{\beta}$$

- P is a positive, real, normalised distribution function over the n-subsystem coherent states $|\ \boldsymbol{\alpha}>$, $|\ \boldsymbol{\beta}>$.

- P exists for any quantum state.

- When appropriate boundary terms vanish, P obeys a Fokker-Planck equation. (FPE)

- The FPE leads to $2n$ complex stochastic equations

Advantages of Positive P

For n subsystems:

- *IMMENSE* improvement over direct solution of density matrix:
  - Density matrix methods would require $2D^n$ real equations, with D itself large.
  - Positive P requires only $4n$ real stochastic equations!
- Used already to make some successful many-body predictions
  - Quantum soliton behaviour in optical fibers [*Nature* **365**, pp 307]
  - Condensation of a BEC [*Phys. Rev. A* **60**, pp R2261]

Anharmonic $\hat{n}^2$ Hamiltonian

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

Is the crucial term for a BEC simulation. Standard Positive P simulations notoriously give unmanageable sampling errors after short times.

The density matrix $\hat{\rho}$ evolves according to

$$\begin{aligned}\frac{\partial\hat{\rho}}{\partial t} &= \frac{-i}{\hbar}[\hat{H},\hat{\rho}] \\ &= \int P(\alpha,\,\beta)\,\frac{\hat{H}\hat{\Lambda}-\hat{\Lambda}\hat{H}}{\mathrm{Tr}[\,\hat{\Lambda}\,]}\,d^2\alpha d^2\beta\end{aligned}$$

with

$$\hat{\Lambda} = ||\alpha><\beta||$$

In terms of the un-normalised Bargmann coherent states

$$||\,\alpha> \quad = \quad e^{\alpha\hat{a}^\dagger}|\,0> = e^{|\alpha|^2/2}|\alpha>$$

We can use the operator identities

$$(\hat{a}^\dagger \hat{a})\,\hat{\Lambda} = \alpha \frac{\partial}{\partial \alpha}\hat{\Lambda}$$

$$\hat{\Lambda}\,(\hat{a}^\dagger \hat{a}) = \beta^* \frac{\partial}{\partial \beta^*}\hat{\Lambda}$$

To generate a Fokker-Planck Equation for P if appropriate boundary terms vanish.

$$\begin{aligned}\frac{\partial P}{\partial t} &= \left[i\frac{\partial}{\partial \alpha}\alpha(\alpha\beta^* + \frac{1}{2}) - i\frac{\partial}{\partial \beta^*}\beta^*(\alpha\beta^* + \frac{1}{2}) \right. \\ &+ \left. \frac{\partial^2}{\partial \alpha^2}\alpha^2 - \frac{\partial^2}{\partial {\beta^*}^2}{\beta^*}^2 \right] P\end{aligned}$$

This then leads to two complex stochastic equations with two real, gaussian noises dW and $d\overline{W}$ with $< dW(t)dW(t') >= \delta(t-t')dt$

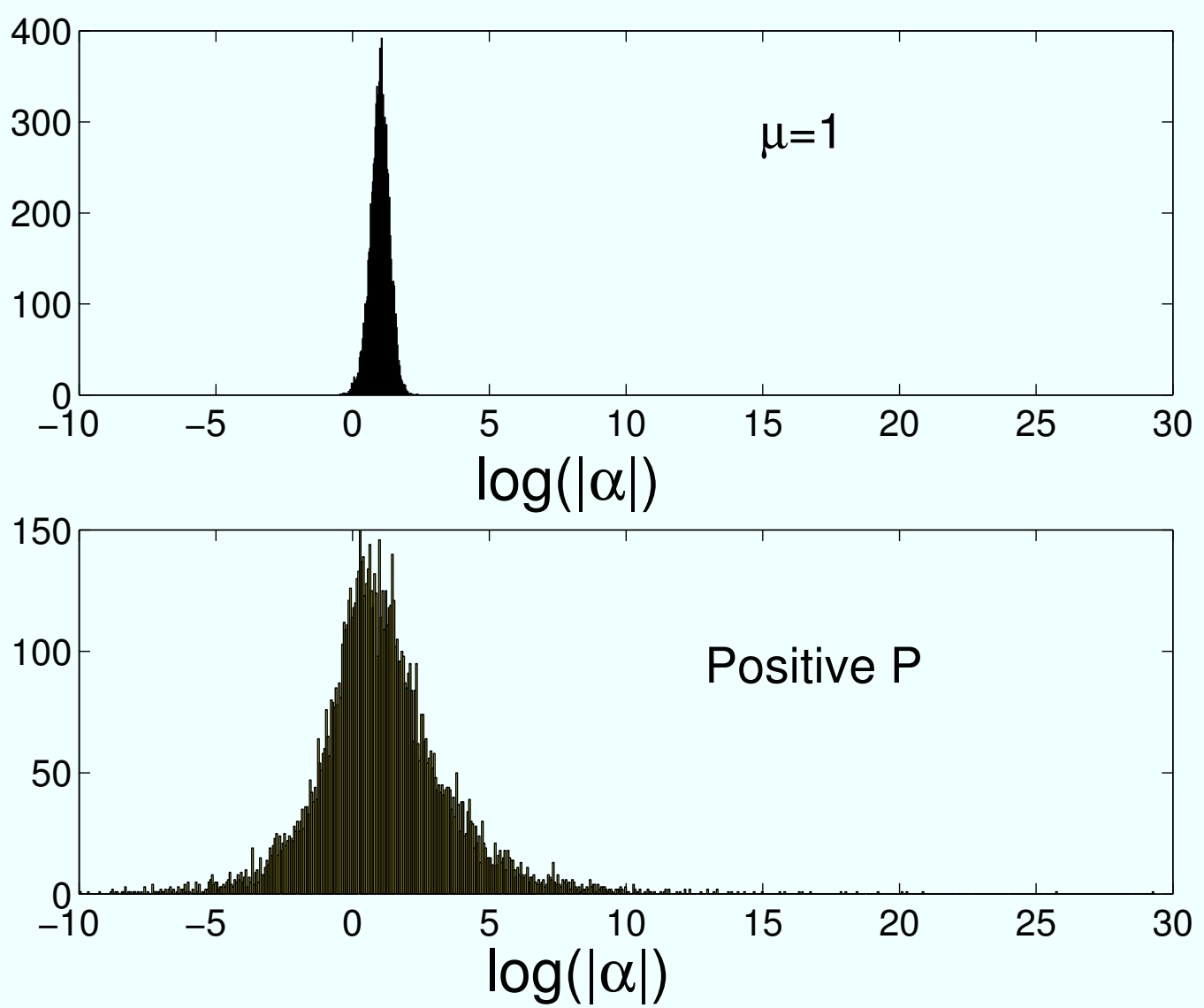
$$\begin{aligned} d\alpha &= -i\alpha[\ (\alpha\beta^* + \frac{1}{2})dt + \sqrt{i}\,dW\ ] \\ d\beta &= -i\beta[\ (\alpha^*\beta + \frac{1}{2})dt + \sqrt{i}\,d\overline{W}\ ] \end{aligned}$$

Observables are then calculated as appropriate averages over the calculated trajectories.

E.g. occupation number of the mode

$$< \hat{a}^\dagger \hat{a} > = < \alpha\beta^* >_{\text{trajectories}}$$

Unfortunately for this hamiltonian (and thus the BEC), the distribution of $|\alpha|$ develops exponentially growing tails after some time. For BECs this occurs at the same time as condensation.



Comparison of the variable α for the positive P and $\mu = 1$ low sampling error gauge. The initial coherent state $\mid 3 >$ was acted on by $\hat{H} = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a})^2$ for $t = 0.6$. *The scale is logarithmic!* Note the small number of very large α values in the Positive P simulation which cause the large sampling error. $10,000$ trajectories shown.

Hermitian P representation

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

The Kernel $\widehat{\Lambda}$ is

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

In terms of n-subsystem Bargmann coherent states

$$||\ \boldsymbol{\alpha} > \quad = \quad \exp\left[\ \sum_{i=1}^{n} \alpha_i \widehat{a}_i^{\dagger}\ \right]\ |\ 0 >$$

- Has all the desirable properties of the Positive P distribution,

- but also addresses the sampling error problem!

- The kernel $\hat{\Lambda}$ consists of coherent states, like the Positive P, but is hermitian.

- $\hat{\Lambda}$ Has an internal quantum phase θ.

- $\hat{\Lambda}$ is entangled if $\boldsymbol{\alpha} \neq \boldsymbol{\beta}$.

- A positive, real P exists for all quantum states.

  $$P(\boldsymbol{\alpha}, \boldsymbol{\beta}, \theta) \quad = \quad P_+(\boldsymbol{\alpha}, \boldsymbol{\beta})\, \delta\left(\theta - \arg(\boldsymbol{\alpha}^* \cdot \boldsymbol{\beta})\right)$$

  (here P_+ is the "old" positive P distribution function.)

- For n subsystems/modes, we would now have $4n + 1$ real stochastic equations. (There is only one quantum phase θ for the entire system.)

- The expectation values of all the observeables can be calculated by generating some amount N of realizations of these stochastioc equations, and averaging over them. To get the expectation value of observable $\hat{X}$

$$< \hat{X} > \quad = \quad \left\langle \frac{\mathrm{Tr}[\hat{X}\hat{\Lambda}]}{\mathrm{Tr}[\ \hat{\Lambda}\ ]} \right\rangle$$

For our anharmonic Hamiltonian

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

We get exactly the same stochastic equations as with the original Positive P distribution.

So, what have we gained..?

Stochastic *Gauges*

With the new kernel, we have new operator identities!

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

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

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

Thus we can add any *arbitrary* multiple, or integral $f, \overline{f}$ of them to the master equation, which contains things like $\int P\hat{H}\hat{\Lambda}$. We can add any functions of the variables: $f(\alpha, \beta, \theta)$ like

$$0 = \int P\, f \left(\frac{\partial^2}{\partial\theta^2} + 1\right) \hat{\Lambda}\, d^2\alpha\, d^2\beta\, d\theta$$

.

Then we obtain correspondences in the Fokker Planck eqn., e.g.

$$0 \;\leftrightarrow\; \left(2\frac{\partial}{\partial\theta} f \tan\left(\theta + \mathrm{Im}[\alpha\beta^*]\right) + \frac{\partial^2}{\partial\theta^2} f\right) P$$

which overall lead to modifications of the stochastic equations.

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

with

$$\tilde{\theta} = \theta + \mathrm{Im}[\alpha\beta^*] \qquad ; \qquad T = \tan(\tilde{\theta})$$

We now have *ARBITRARY* functions (*Gauges*) $G, \bar{G}$ in the stochastic equations which we can use to tailor them our satisfaction!

- The choice $G = \bar{G} = 0$ gives the "old" positive P equations.

  ($G = f - \frac{1}{2}\,\mathrm{Re}[\,\alpha\beta^*(1+i)\,]$, etc.)

- Our aim is to reduce sampling error. We do this by keeping α and β fairly small – this causes diffusion in the $\tilde{\theta}$ variable. A gauge which achieves very small sampling error is

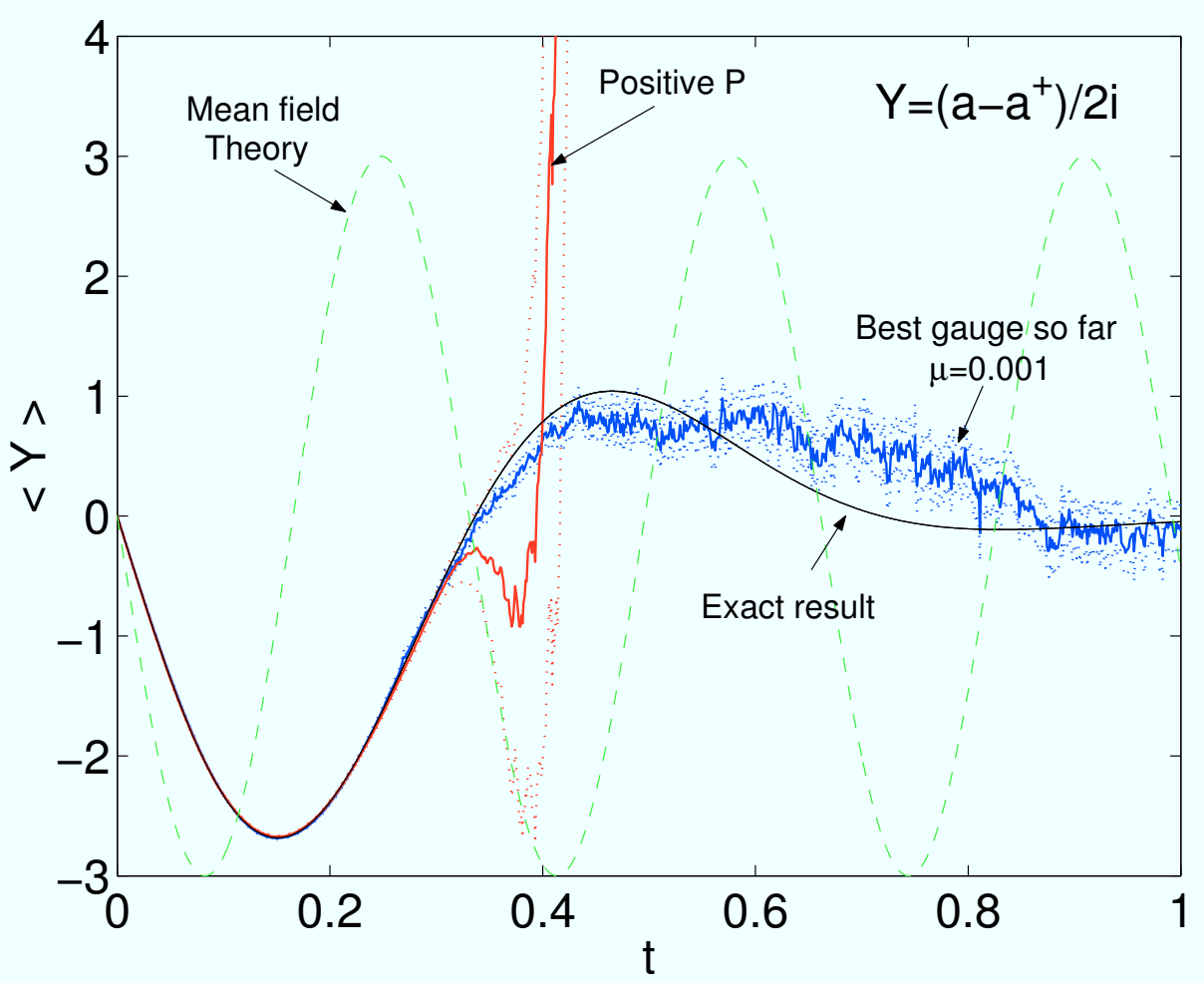
$$G = \tfrac{1}{2}\left(|\alpha|^2 - \mathrm{Re}[\alpha\beta^*(1+i)]\right)$$

$$\bar{G} = \tfrac{1}{2}\left(|\beta|^2 + \mathrm{Re}[\alpha\beta^*(1-i)]\right)$$

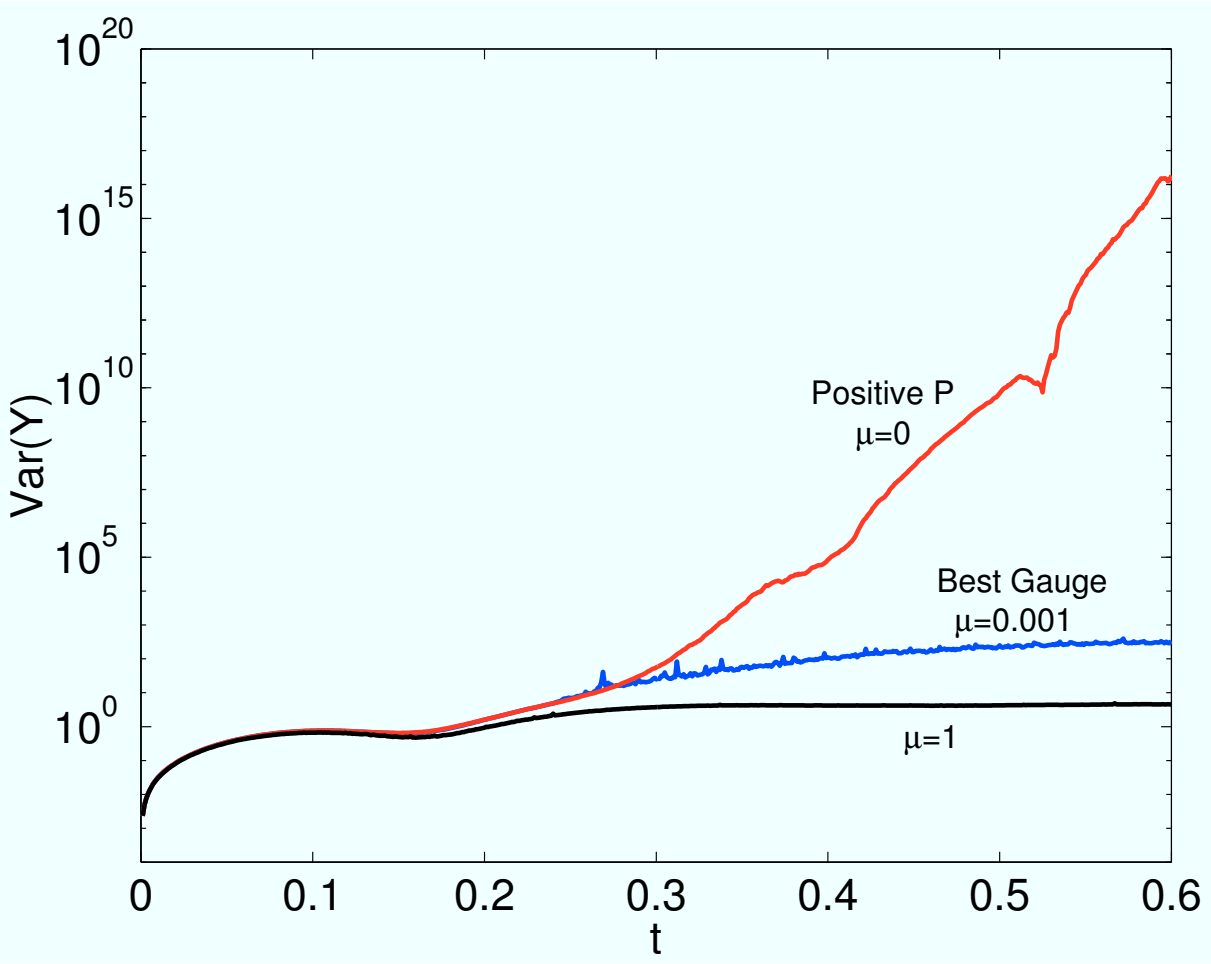
- Unfortunately, this particular gauge appears to lead to non-vanishing boundary terms in the $\tilde{\theta}$ variable, which gives some (reasonably small) systematic errors in the resulting observables.

- If we make the departure from the "old" positive P behaviour small, by multiplying the above gauges by a constant factor μ, then these systematic errors become negligible for most time frames, while the sampling error is still very small compared to the positive P simulation. There appears to be a tradeoff between boundary terms and sampling error.

- For the trial case we have been investigating ($\alpha(0) = \beta(0) = 3$), $\mu = 0.001$ 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. Dotted lines indicate the size of the errors due to finite sampling.



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 $(\widehat{n})^2$ 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!

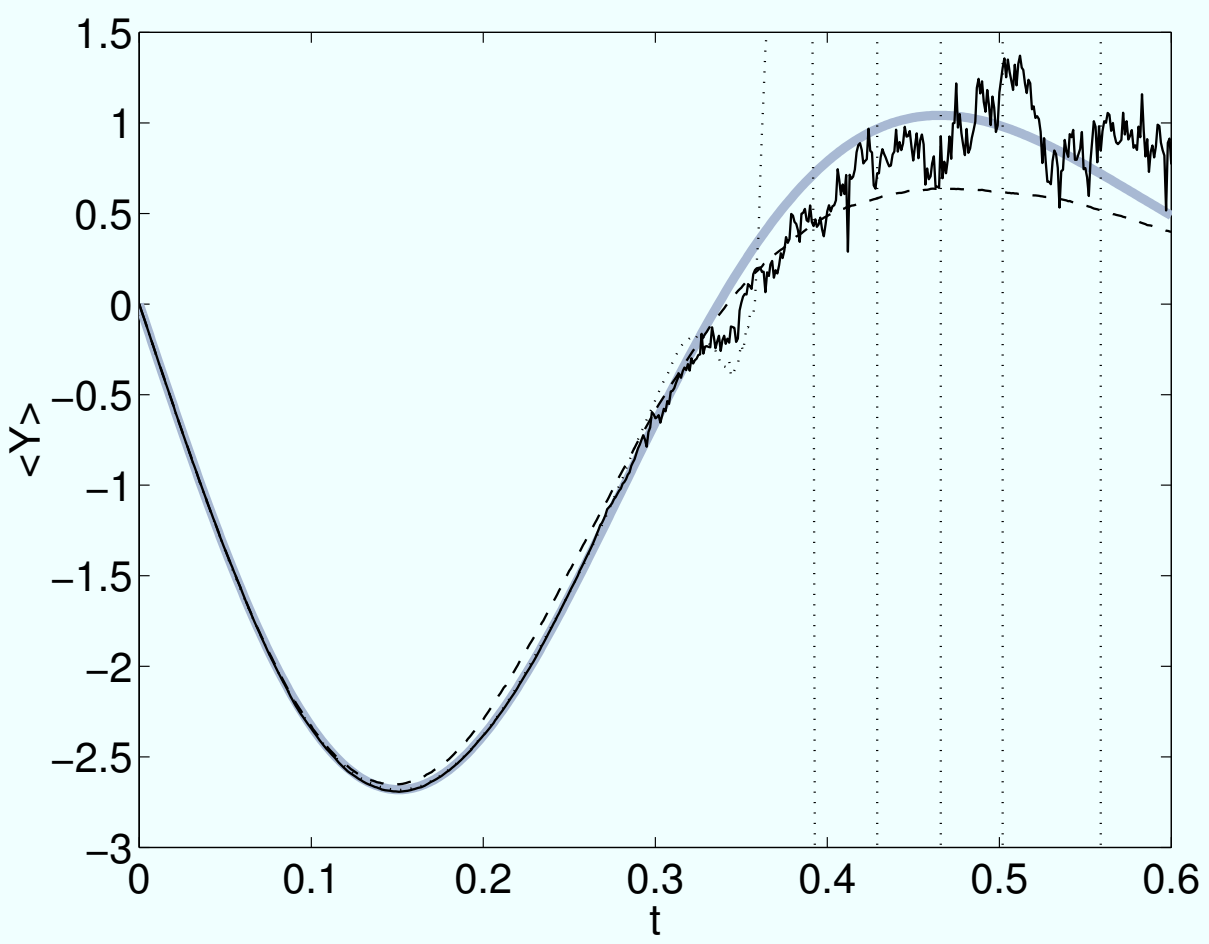
- When the last "kinks" are ironed out of this method, it should be possible to perform full quantum simulations of BEC's.

- Further investigation needed to optimize the gauge – i.e. remove the boundary term "kinks".

- 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



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. Thick shaded line: exact result; Dotted line: Positive P distribution; Dashed line: $\mu = 1$ Hermitian gauge; Solid line: $\mu = 0.001$ hermitian gauge.