Stochastic Gauges in quantum dynamics for many-body simulations

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- "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)

- We need to improve on methods already implemented by the Positive P, and other quasi-probability representations.

Positive P representation

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

- 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]
- Already well understood.

Drawbacks of Positive P

- For many interesting systems,
  sampling error becomes unmanageable in finite time.

- Requires boundary terms in phase space to vanish.

- Not exact for high order interactions. ($>$3rd order in $\hat{a}^\dagger$)
  Fortunately, this is insignificant in many interesting cases.

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:

$$\begin{aligned}
\hat{H} &= \int d^d\mathbf{x}\left[\frac{\hbar^2}{2m}\nabla\hat{\Psi}^\dagger(\mathbf{x})\nabla\hat{\Psi}(\mathbf{x}) + V(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\right] \\
&+ \int d^d\mathbf{x}\left[\hat{\Psi}^\dagger(\mathbf{x})\hat{R}(\mathbf{x}) + \hat{\Psi}(\mathbf{x})\hat{R}^\dagger(\mathbf{x})\right] \\
&+ \frac{1}{2}\int\int d^d\mathbf{x}d^d\mathbf{y}U(\mathbf{x}-\mathbf{y})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{y})\hat{\Psi}(\mathbf{y})\hat{\Psi}(\mathbf{x})\,.
\end{aligned}$$

Simplified lattice model (ignoring reservoirs)

- Generic interaction Hamiltonian of a lattice Bose gas,
- Nonlinear interactions between the sites
- linear interactions that couple different sites together:

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

$+$ trap potential, damping, noise

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

- 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 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. (See figures 1, 2, 4).

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

- Have found one. See below!

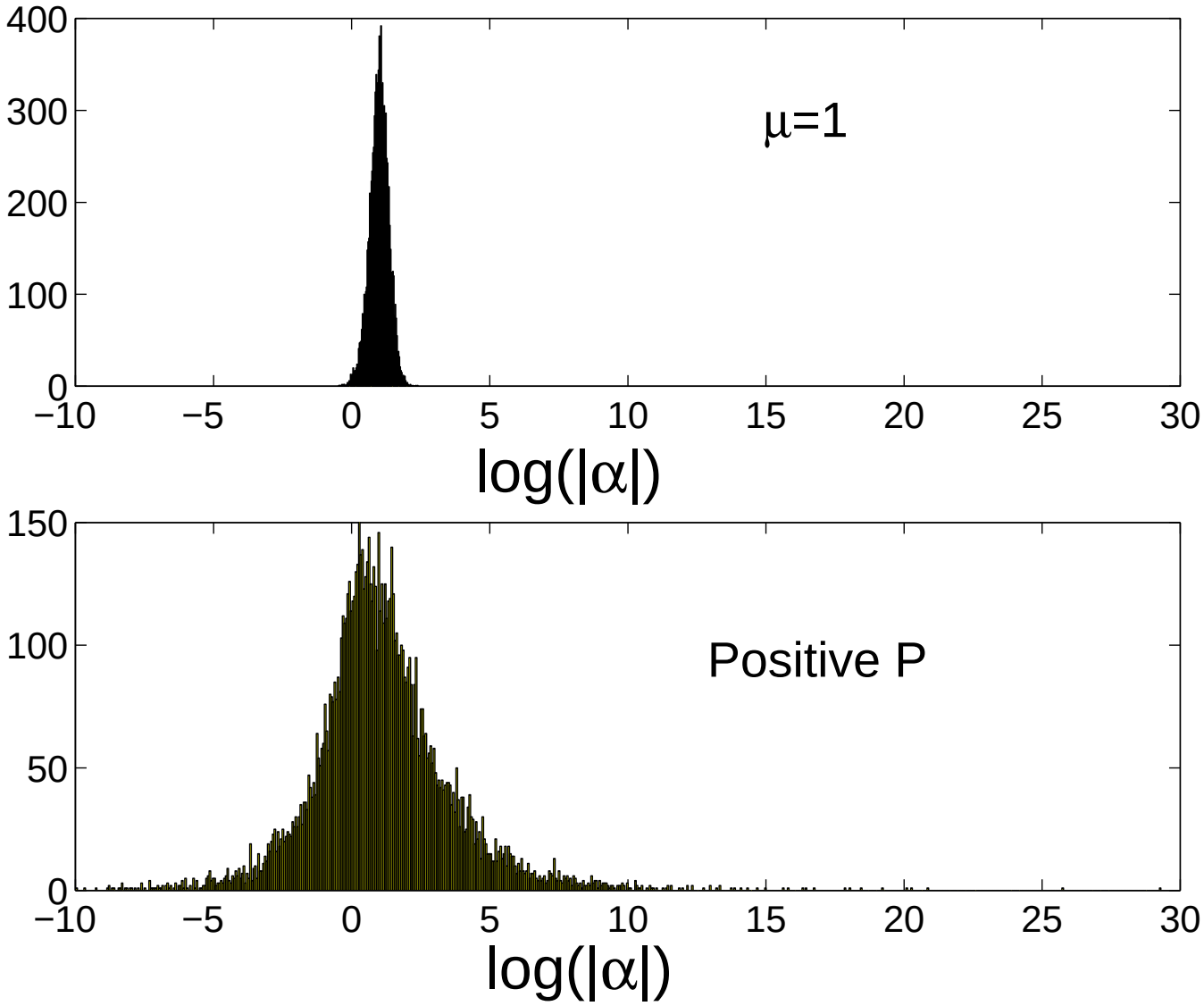

Figure 1: Comparison of the variable α for the positive P and $\mu = 1$ low sampling error gauge. The initial coherent state $\mid 3 >$ was acted on by $\hat{H} = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a})^2$ for $t = 0.6$. *The scale is logarithmic!* Note the small number of very large α values in the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

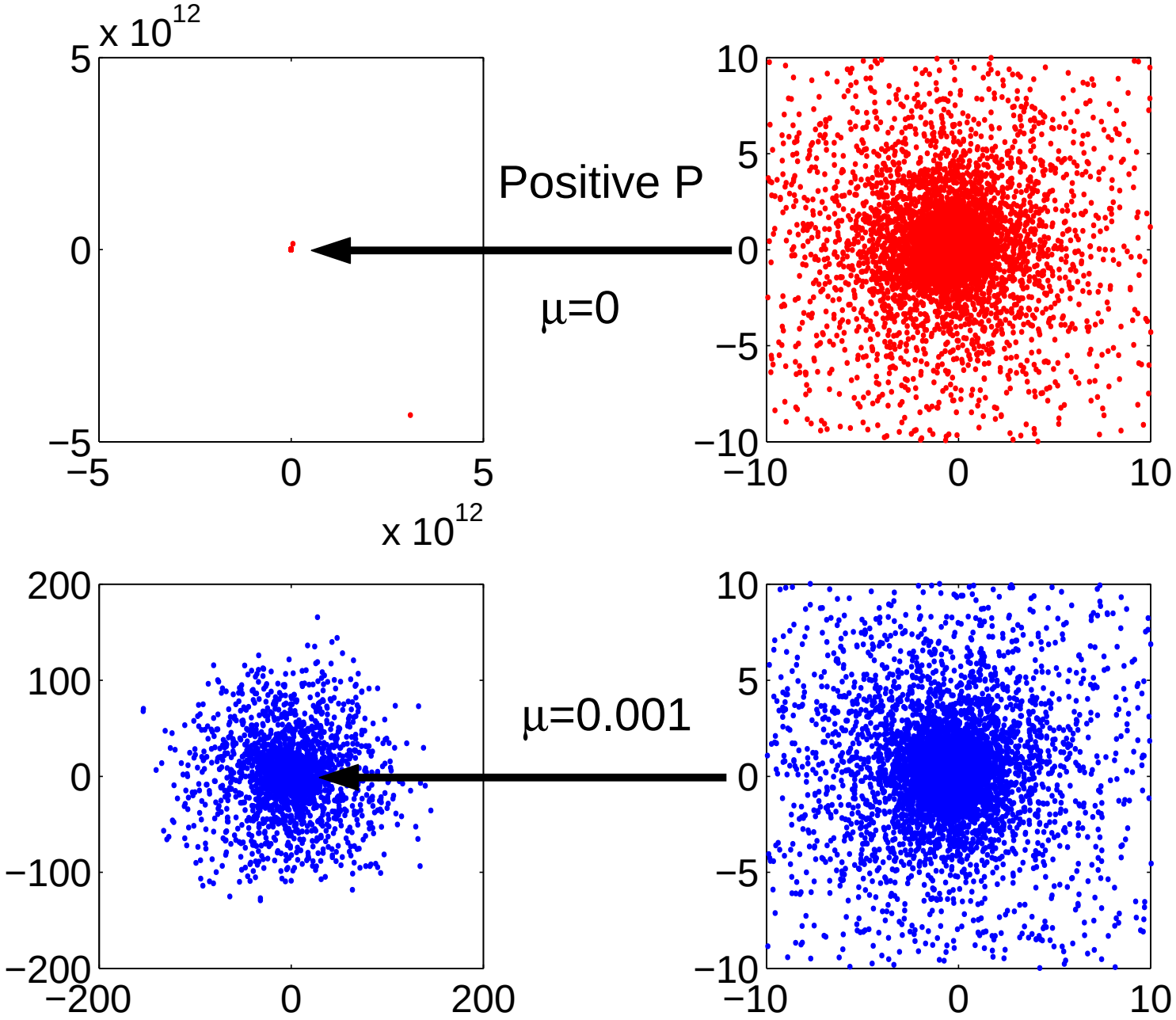

Figure 2: Comparison of the variable α for the positive P and $\mu = 0.001$ optimum gauge after $t = 0.6$. $10,000$ trajectories shown.

Hermitian P representation

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

The Kernel $\hat{\Lambda}$ is

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

In terms of n-subsystem Bargmann coherent states

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

- 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 $\hat{X}$

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

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 (see figure 4).

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

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

We can use the operator identity

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

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

This then leads to two complex stochastic equations with two real noises dW and $d\overline{W}$. In fact, the same ones as for the Positive P!

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

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 $f, \overline{f}$ of them to the master equation! This includes functions of the variables: $f(\alpha, \beta, \theta)$.

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

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

which overall lead to modifications of the stochastic equations.

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

with

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

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. (See figures 3 and 4).

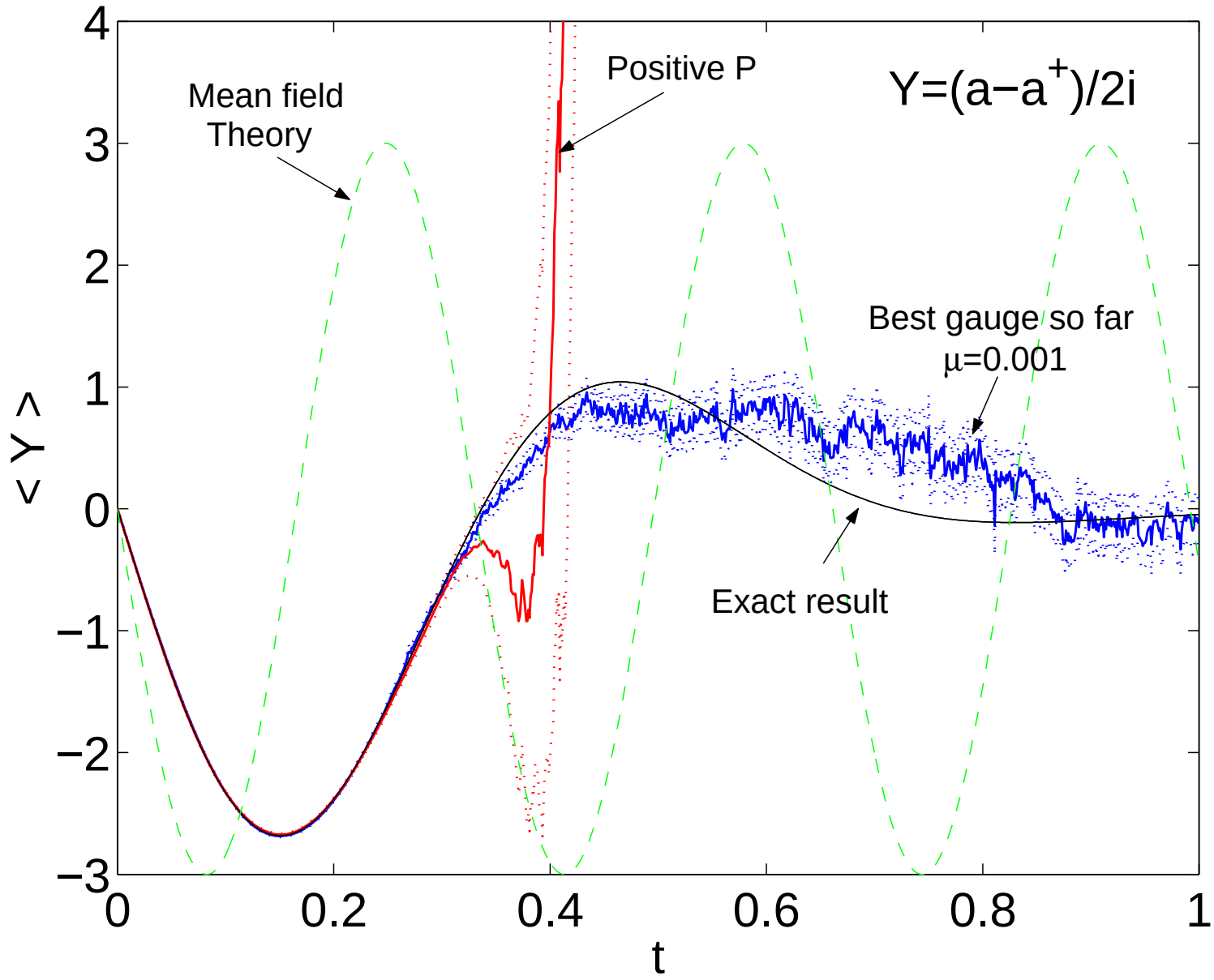

Figure 3: Comparison of simulations of the quadrature $\hat{Y} = \frac{1}{2i}(\hat{a} - \hat{a}^\dagger)$ for an initial coherent state $\mid 3 >$ acted on by $\hat{H} = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a})^2$. $10,000$ trajectories. Dotted lines indicate the size of the errors due to finite sampling.

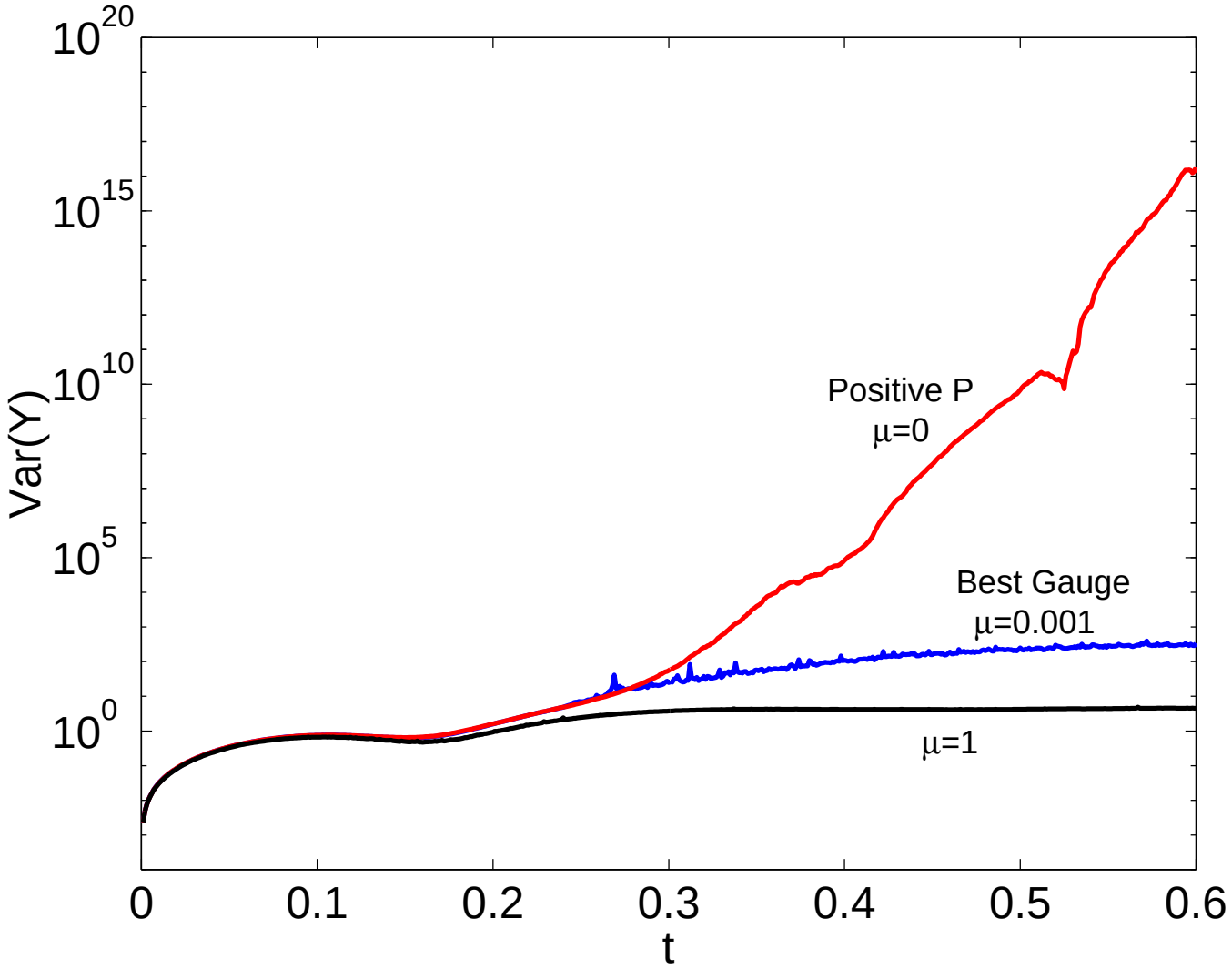

Figure 4: Comparison of sampling errors for various stochastic simulations: "old" positive P ($\mu = 0$), small sampling hermitian P ($\mu = 1$), best hermitian P ($\mu = 0.001$). Shown is the variance in quadrature $\hat{Y}$. Size of actual sampling uncertainty in calculated moment for N trajectories 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.

- 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.