Phase-space methods for quantum simulations

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The problem: complexity

How can we calculate quantum dynamics?

BEC: 10^{100000} **states,** 10^6 **qubits in Hilbert space**

✘ Real time path integrals **don't converge**

✘ Mean field methods **don't give quantum statistics**

✘ Direct computation needs **don't fit into memory**!

Phase-space representations

✔ Quantum dynamics $\longrightarrow$ stochastic motion + sampling

✘ **Classical** phase-space: **Wigner, P-, Q**, d dimensions

✔ **Quantum** phase-space: **Positive-P**, $2d$ dimensions

✔ Stochastic gauge: adds a weight to the trajectory

Phase-Space Representations

Expand the density matrix $\widehat{\rho}$, using operators $\widehat{\Lambda}(\overrightarrow{\lambda})$:

$$\widehat{\rho} = \int P(\overrightarrow{\lambda})\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda}$$

Quantum dynamics $\longrightarrow$Trajectories in $\overrightarrow{\lambda}$.

Different basis choice $\widehat{\Lambda}(\overrightarrow{\lambda})$ $\longrightarrow$different representation

General M-mode Gaussian operator

Normally-ordered exponential of a general quadratic form in the $2M$-vector mode operator $\delta\underline{\widehat{a}} = (\widehat{\mathbf{a}}, \widehat{\mathbf{a}}^{\dagger}) - \underline{\alpha}$, where $\underline{\alpha}$ is a $2M$-vector c-number and $\widehat{\mathbf{a}}$ is the vector of annihilation operators. For algebraic reasons, it is useful to employ normal ordering, and to introduce a compact notation using a generalized covariance $\underline{\underline{\sigma}}$:

$$\widehat{\Lambda}(\overrightarrow{\lambda}) = \frac{\Omega}{\sqrt{\left|\underline{\underline{\sigma}}\right|}} : \exp\left[-\delta\underline{\widehat{a}}^{\dagger}\underline{\underline{\sigma}}^{-1}\delta\underline{\widehat{a}}/2\right] : \ .$$

In this case, the phase-space is described by the complex variables $\overrightarrow{\lambda} = (\Omega, \underline{\alpha}, \underline{\underline{\sigma}}) = (\Omega, \alpha)$.

What is the covariance?

$$\underline{\underline{\sigma}} = \begin{bmatrix} \mathbf{I}+\mathbf{n} & \mathbf{m} \\ \mathbf{m}^{+} & \mathbf{I}+\mathbf{n}^{T} \end{bmatrix} .$$

The representation phase space is $\overrightarrow{\lambda} = (\Omega, \alpha, \alpha^{+}, \mathbf{n}, \mathbf{m}, \mathbf{m}^{+})$

- Ω= weight factor
- $\alpha, \alpha^{\dagger}$= amplitude
- $\mathbf{n}$ = number correlation (complex $M \times M$ matrix).
- $\mathbf{m}, \mathbf{m}^{+}$= squeezing (symmetric complex $M \times M$ matrices)

What are the moments physically?

$$
\begin{aligned}
\langle \widehat{a}_i \rangle &= \langle \Omega \alpha_i \rangle_P \\
\left\langle \widehat{a}_i^{\dagger} \right\rangle &= \langle \Omega \alpha_i^{+} \rangle_P \\
\langle \widehat{a}_i \widehat{a}_j \rangle &= \langle \Omega (\alpha_i \alpha_j + m_{ij}) \rangle_P \\
\left\langle : \widehat{a}_i \widehat{a}_j^{\dagger} : \right\rangle &= \langle \Omega (\alpha_i \alpha_j^{+} + n_{ij}) \rangle_P \\
\left\langle \widehat{a}_i^{\dagger} \widehat{a}_j^{\dagger} \right\rangle &= \langle \Omega (\alpha_i^{+} \alpha_j^{+} + m_{ij}^{+}) \rangle_P \; .
\end{aligned}
$$

Standard Phase-space Representations

What about the text-book phase-space representations?

Property: **Repn.**	***Variance*** (n)	***Operator Order***	**Phase-space**
P	0	Normal	Classical
W	1/2	Symmetric	Classical
Q	1	Antinormal	Classical
+P	0	Normal	Classical$\times 2$
G	n	**Any**	$($Classical$)^2$

TYPES OF PROBLEM

There are three main types of problems studied:

- ✔ Master equations - damping + coherent evolution
- ✔ Canonical ensembles - ‘imaginary time’ thermal equilibrium
- ✔ Quantum dynamics - purely coherent nonlinear evolution

OUTLINE

1. **PROBLEM:** $\partial\widehat{\rho}/\partial t = \widehat{L}[\widehat{\rho}]$

2. Define: p-dimensional complex space: $\overrightarrow{\lambda} = (\Omega, \alpha)$

3. **Basis** $\widehat{\Lambda}(\overrightarrow{\lambda})$: $\widehat{\rho} = \int P(\overrightarrow{\lambda})\widehat{\Lambda}(\overrightarrow{\lambda})d^{2p)}\overrightarrow{\lambda}$

4. Identities: $\partial\widehat{\rho}/\partial t = \int P(\overrightarrow{\lambda})\mathcal{L}_A\widehat{\Lambda}(\overrightarrow{\lambda})d^{2p}\overrightarrow{\lambda}$

5. **Diffusion and drift gauge**: $\mathbf{g}^d(\alpha), \mathbf{g}(\alpha)$

6. **STOCHASTICS:**
$$d\Omega/\partial t = \Omega\,[U + \mathbf{g}\cdot\zeta]$$
$$d\alpha/\partial t = \mathbf{A} + \mathbf{B}(\zeta - \mathbf{g})$$

CENTRAL RESULT

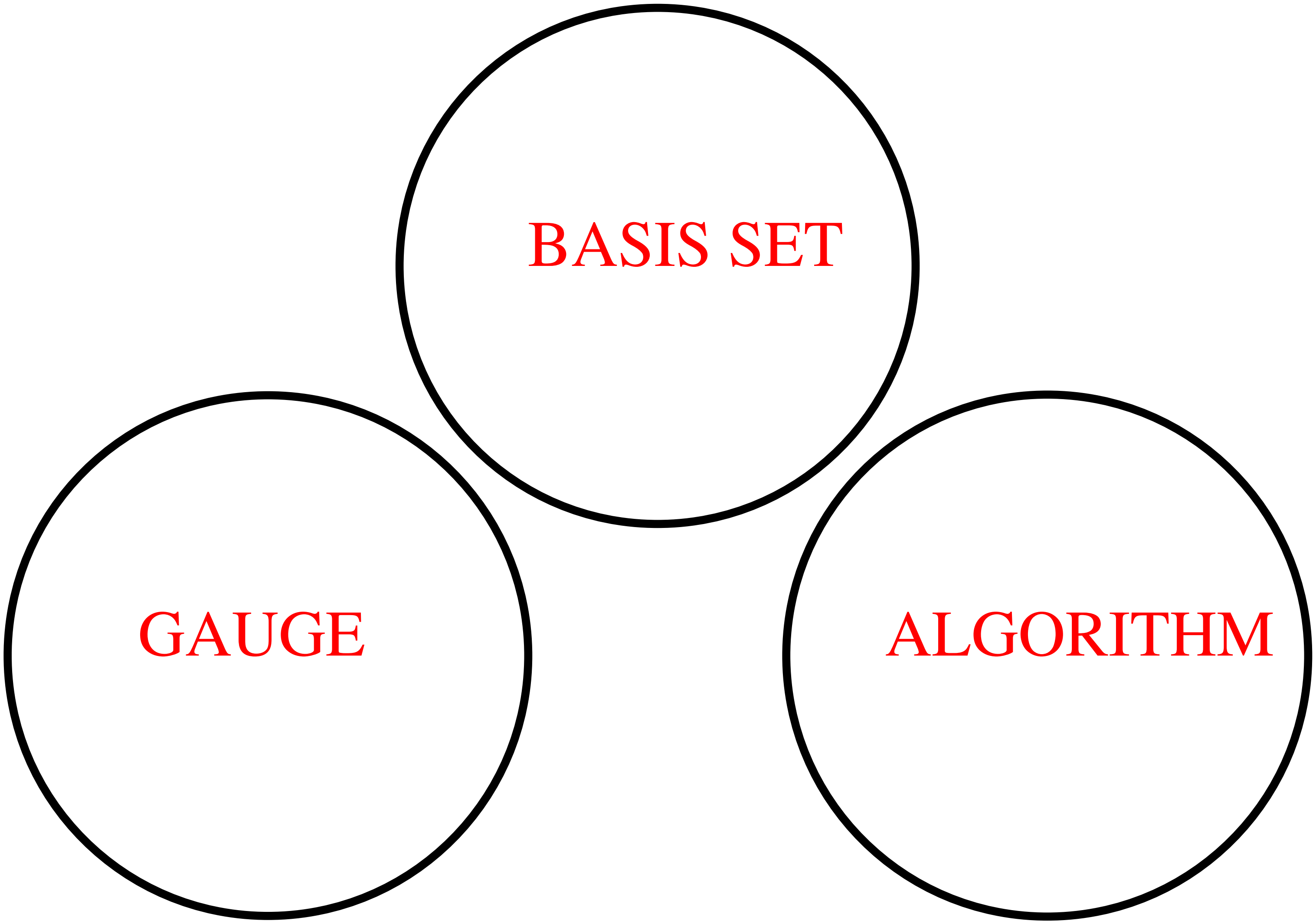
Stochastic equations: **trajectory** α, quantum **amplitude** Ω:

Gauge $$d\Omega/\partial t = \Omega\left[U dt + \mathbf{g}(\alpha)\cdot\zeta(t)\right]$$

Trajectory $$d\alpha/\partial t = \mathbf{A} + \mathbf{B}\left[\zeta(t) - \mathbf{g}(\alpha)\right]$$

- Noise correlations: $\langle \zeta_i(t)\zeta_j(t')\rangle = \delta_{ij}\delta(t-t')$
- Gauges chosen freely to optimize simulations
- Provided no boundary terms, all gauges EQUIVALENT
- Works for either bosons or fermions
- Sign changes for fermions and NO amplitude terms

COMPUTATIONAL STRATEGIES



League Table of Representations

How do the known phase-space representations compare?

Property: **Repn.**	*Finite?*	*2nd Order*	*Pos. Def.?*	*SDE ?*	*Stable?*
P	No	-	-	-	-
W	Yes	No	-	-	-
R	Yes	Yes	No	-	-
Q	Yes	Yes	Yes	No	-
+P	Yes	Yes	Yes	Yes	No
G	**Yes**	**Yes**	**Yes**	**Yes**	**Yes**

I: CANONICAL BOSE-HUBBARD MODEL

Nonlinear interactions at each site + linear interactions coupling different sites:

- $\widehat{H}(\mathbf{a},\mathbf{a}^{\dagger}) = \hbar\left[\sum\sum\omega_{ij}a_i^{\dagger}a_j + \sum :\widehat{n}_j^2:\right]$.
- ω_{ij} - nonlocal coupling, includes chemical potential.
- Boson number: $\widehat{n}_i = a_i^{\dagger}a_i$.
- Grand canonical ensemble: $\hat{\rho}_u = e^{-(\hat{H}-\mu\hat{N})/k_BT} = e^{-\hat{K}\tau}$.

Stochastic gauge equations

Choose $n = 0$ *then* $\rightarrow$ *Imaginary time* Gross- Pitaevskii equations with **weighting** and **quantum noise**:

$$\frac{d\alpha_i}{d\tau} = -\left[\alpha_i^\dagger \alpha_i + i g_i\right]\alpha_i - \sum_{j=1}^{M} \omega_{ij}\alpha_j/2 + i\alpha_i\zeta_i(\tau)$$

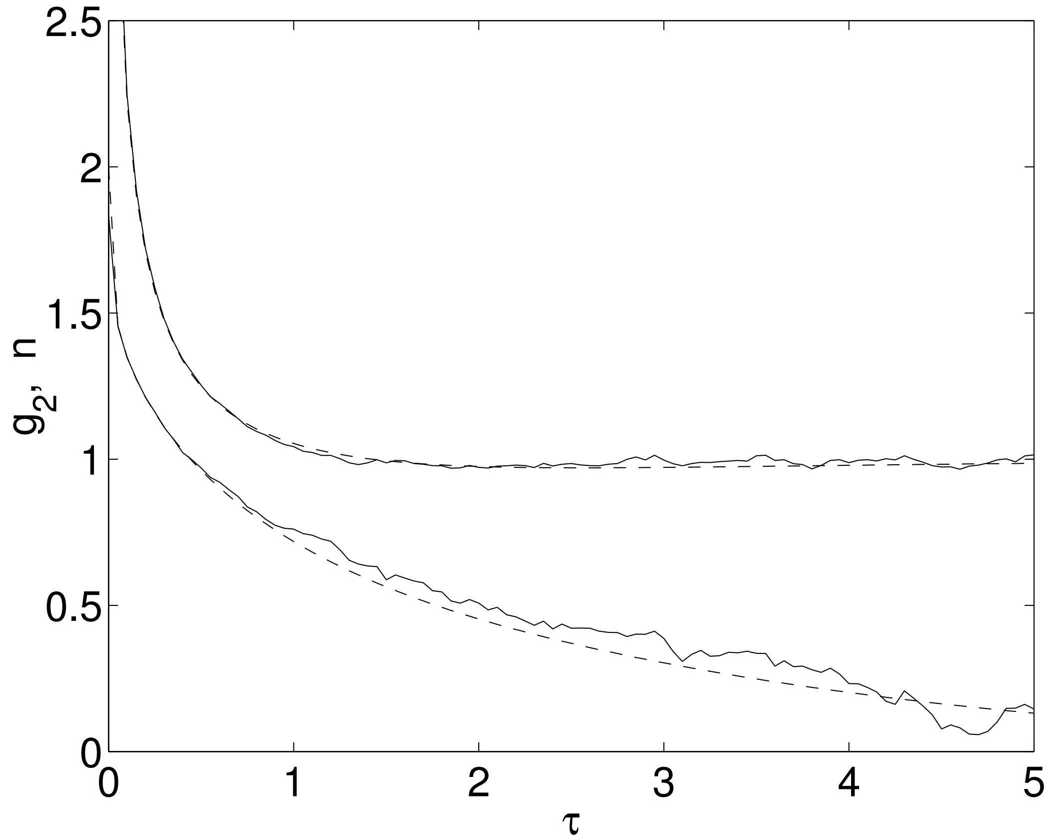
$$\frac{d\Omega}{d\tau} = \left[-K(\tau)d\tau + \sum_{i=1}^{M} g_i\zeta_i(\tau)\right]\Omega$$

STABILISING GAUGE: $g_j = i(Re(\alpha_i^\dagger\alpha_i) - |\alpha_i^\dagger\alpha_i|)$,

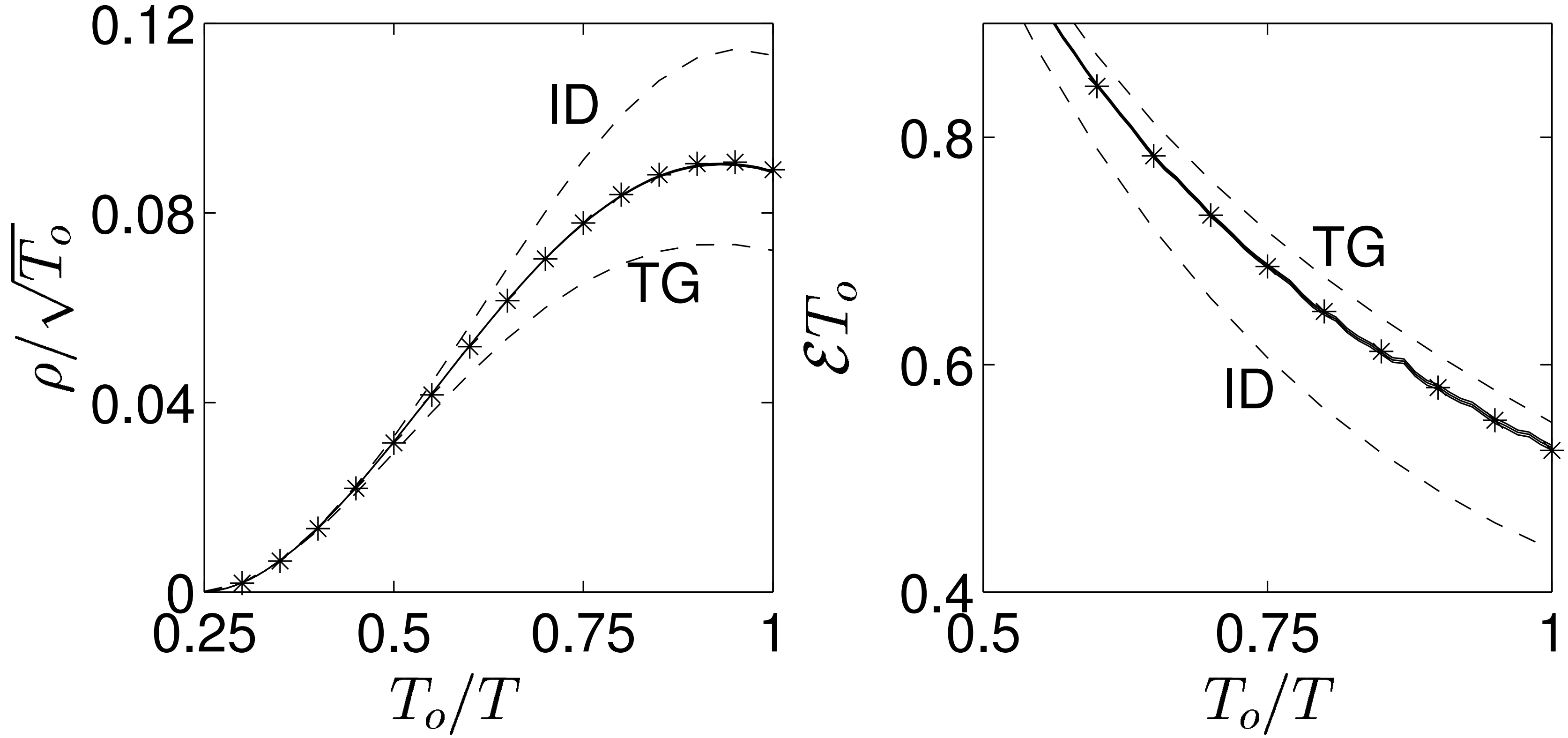
Single-well, interacting case

Antibunching: single Bose mode,

NOTE: $\tau =$Inverse temperature



Simulations vs exact energy and density

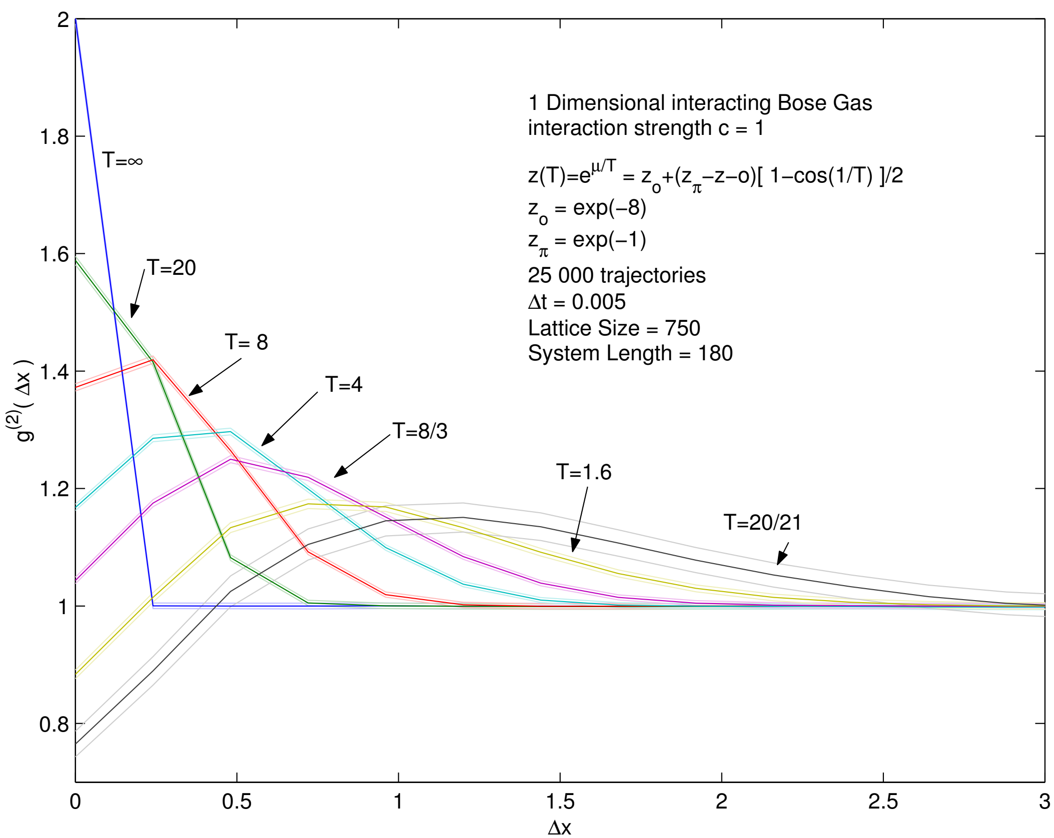


✔ Complete agreement with exact solutions

- at all temperatures calculated!

Spatial correlations

Spatial correlations, $g^{(2)}(x)$ can be calculated from gauge simulations:



II: REAL-TIME BOSE-HUBBARD MODEL

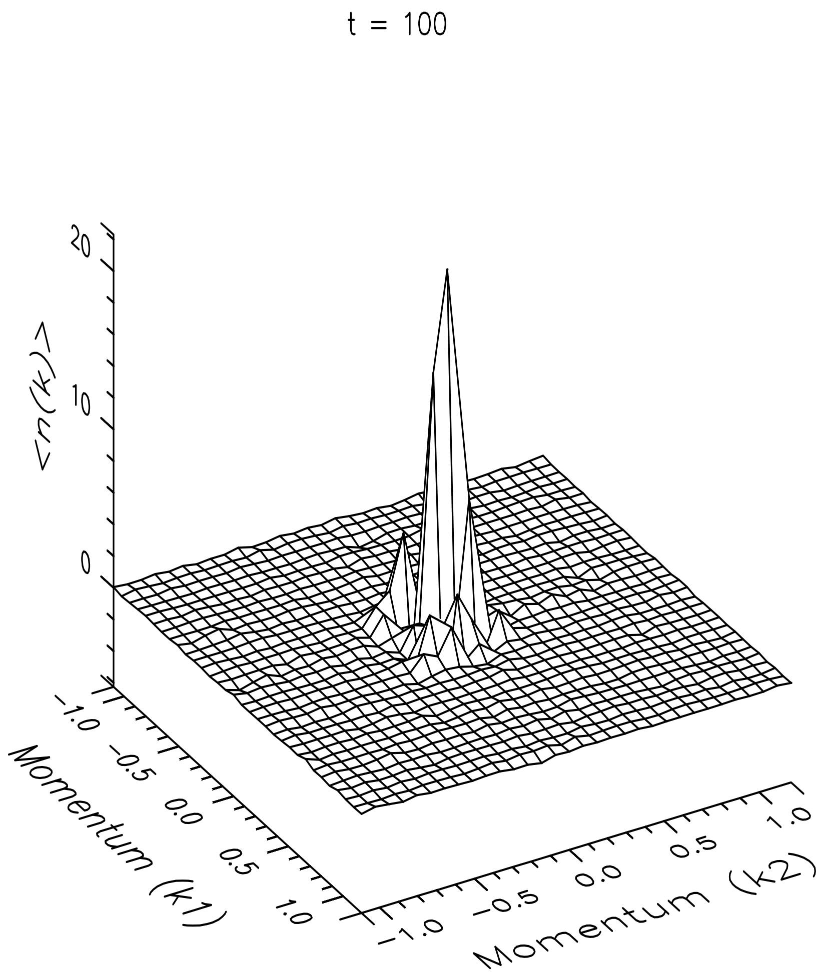
- $n = 0$ *(positive-P)* $\rightarrow$ *Real time* Gross- Pitaevskii equations with **quantum noise**:

$$\frac{d\alpha_i}{dt} = -i\left[n_i + \sum_{j=1}^{2M}\omega_{ij}\alpha_j + \sqrt{i}\zeta_i(\tau)\right]\alpha_i$$

- $n = 1/2$ *(Wigner)* $\rightarrow$ *Approximate* Gross- Pitaevskii equations with $\langle\alpha_i^{0*}\alpha_i^0\rangle = 1/2$

$$\frac{d\alpha_i}{dt} = -i\left[n_i + \sum_{j=1}^{2M}\omega_{ij}\alpha_j\right]\alpha_i$$

BEC evaporative cooling (1998): 10^5 qubits



III: NONCLASSICAL QUANTUM DYNAMICS:

Coherent molecular down-conversion

- Coherent process of molecular dissociation
- Overall effective Hamiltonian term in one dimension of

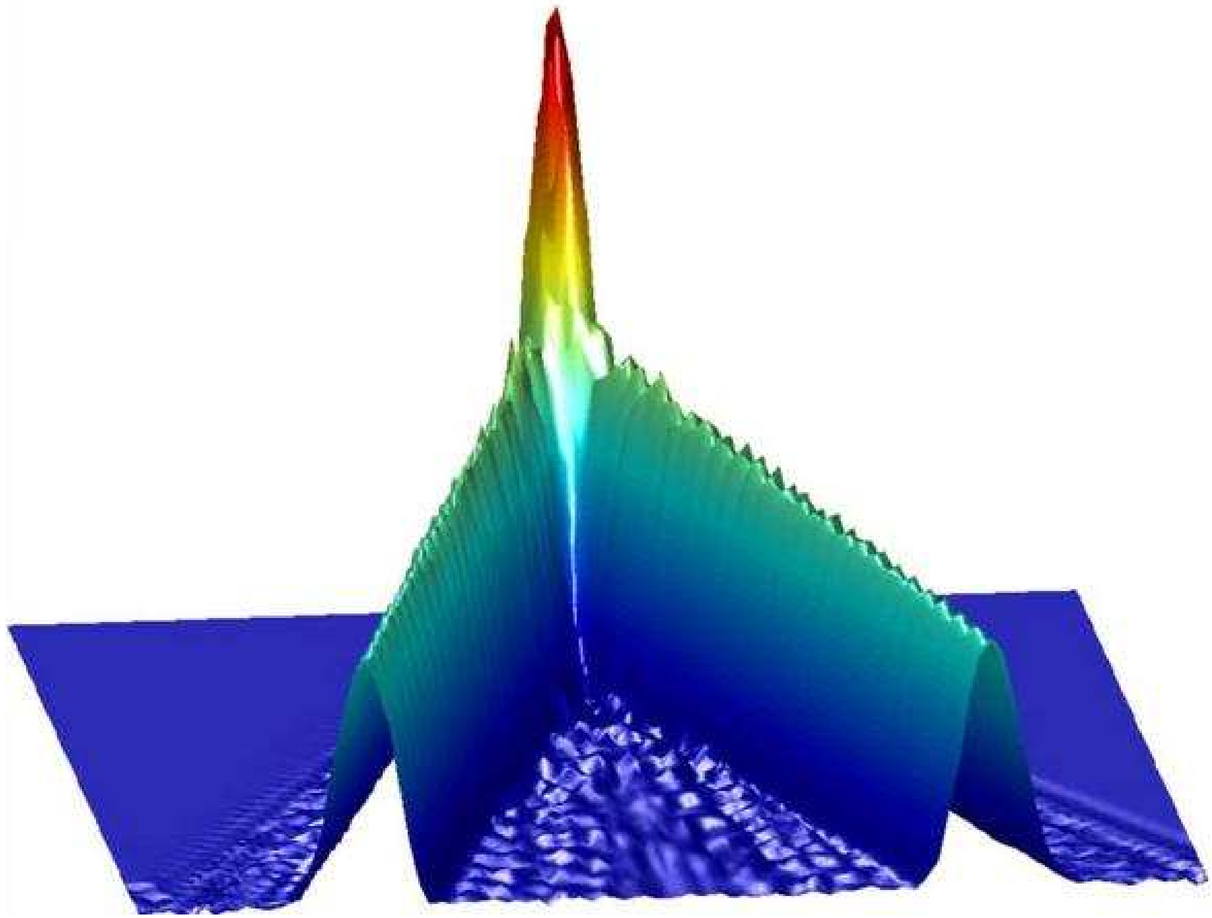
$$\hat{H} = \hat{H}_0 - i\frac{\hbar\chi(t)}{2}\int dx\left[e^{i\omega t}\hat{\Psi}_2^\dagger\hat{\Psi}_1^2 - e^{-i\omega t}\hat{\Psi}_2\hat{\Psi}_1^{\dagger\,2}\right],$$

- $\chi(t)$ is the bare atom-molecule coupling; ω is a detuning

Stochastic Equations

$$
\begin{aligned}
\frac{\partial \psi_1}{\partial \tau} &= i\frac{\partial^2 \psi_1}{\partial \xi^2} - (\gamma + i\delta)\psi_1 + \kappa\psi_2\psi_1^+ + \sqrt{\kappa\psi_2}\eta_1 \, , \\
\frac{\partial \psi_1^+}{\partial \tau} &= -i\frac{\partial^2 \psi_1^+}{\partial \xi^2} - (\gamma - i\delta)\psi_1^+ + \kappa\psi_2^+\psi + \sqrt{\kappa\psi_2}\eta_1^+ , \\
\frac{\partial \psi_2}{\partial \tau} &= \frac{i}{2}\frac{\partial^2 \psi_2}{\partial \xi^2} - iv(\xi,\tau)\psi_2 - \frac{\kappa}{2}\psi_1^2 + \sqrt{-iu}\psi_2\eta_2 \, , \\
\frac{\partial \psi_2^+}{\partial \tau} &= -\frac{i}{2}\frac{\partial^2 \psi_2^+}{\partial \xi^2} + iv(\xi,\tau)\psi_2^+ - \frac{\kappa}{2}\psi_1^{+2} + \sqrt{iu}\psi_2^+\eta_2^+ \, .
\end{aligned}
$$

Twin atom correlations



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