Computational aspects of quantum phase-space methods

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The 2005 Nobel Prize in Physics

The Royal Swedish Academy of Sciences awards the 2005 Nobel Prize in Physics, with one half to

Roy J. Glauber

- ***for his contribution to the quantum theory of optical coherence***

What are coherent states?

These are idealized states which are coherent to all orders! If a is a field operator, then:

$$a\,|\alpha\rangle = \alpha\,|\alpha\rangle$$

- Coherent states are a **complete mathematical basis**
- **Also SU(N) coherent states**
- Examples of states which are perfectly coherent

P-representation

- Coherent states $\longrightarrow$ **quantum operator representations**

$$\widehat{\rho} = \int P(\alpha) \left|\alpha\right\rangle \left\langle\alpha\right| d^2\alpha$$

- Maps quantum states into **classical phase-space**
- Used to develop quantum theory of the laser
- **Glauber, Agarwal, Sudarshan, Lax, Wigner, Husimi..**

Classical phase-space

Early representations used a classical phase-space.

For M modes, and N particles/mode

Usual QM: $\longrightarrow N^M$ (complex) coordinates

Wigner QM$\longrightarrow M$ coordinates

Glauber-Sudarshan$\longrightarrow M$ coordinates

PROBLEM: distributions can have negative or singular values, and obey a complicated differential equation!

SOLUTION: Quantum phase-space

Enlarged phase-space allows quantum superpositions.

Positive-P $2M$ coordinates

$$\widehat{\rho} = \int P(\alpha, \beta) \frac{|\beta\rangle \langle\alpha|}{\langle\alpha| |\beta\rangle} d^2\alpha d^2\beta$$

Distributions are positive and obey a diffusion equation!

Contributors: Drummond, Chaturvedi, Walls, Gardiner.

21st CENTURY: ultracold atoms - the ideal quantum system

- ✔ Bose-Einstein condensates: atom ‘photons’
- ✔ Quantum superfluid Fermi atoms: atom ‘electrons’
- ✔ ‘Superchemistry’; molecule formation from bosons
  - ✔ Atom lasers, atomic diffraction, interferometers..
  - ✔ ULTRALOW temperatures down to $1nK$
  - ✔ TESTS QUANTUM THEORY IN NEW REGIMES!

MANY-BODY QUANTUM DYNAMICS

- many-body problems become exponentially complex.
- consider n atoms distributed among m modes
  - take $n \simeq m \simeq 500,000$:
  - Number of quantum states: $N_s = 2^{2n} = 10^{100,000}$
- **Can't diagonalize Hamiltonian!**

Main Approaches: Quantum time-evolution

- ✘ Traditional methods:
  - ✘ Path integrals - diverging phase problem
  - ✘ Perturbation theory - doesn’t converge
  - ✘ Exact solutions - exponential initial value problem
- ✘ New hardware: Quantum computers - don’t exist?
- ✔ New basis: Gaussian quantum phase-space

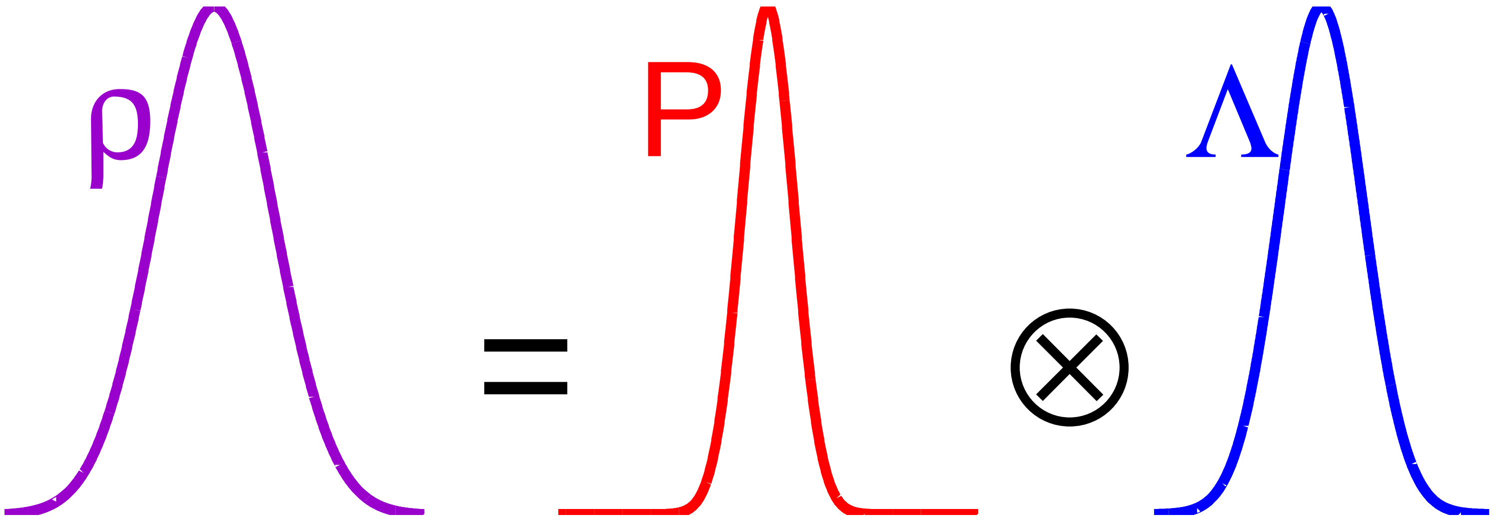
General phase-space representations

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
- P-representation: $\widehat{\Lambda}(\alpha) = |\alpha\rangle\langle\alpha|$

Trade-offs: distribution vs basis



$$\sigma_\rho \sim \sigma_P + \sigma_\Lambda$$

General M-mode Gaussian operator

Normally-ordered exponential of a 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 c-vector and $\widehat{\mathbf{a}}$ is the vector of annihilation operators.

Boson kernel - (similar result for fermions)

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

Quantum phase-space: $\overrightarrow{\lambda} = (\Omega, \underline{\alpha}, \underline{\underline{\sigma}})$.

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
- α, α^{+}= amplitude
- $\mathbf{n}$ = number correlation - OBSERVABLE
- $\mathbf{m}, \mathbf{m}^{+}$= squeezing - OBSERVABLE

Bosonic and fermionic operator identities

$$\left\langle \widehat{a}_i^\dagger \widehat{a}_j \right\rangle = \langle n_{ij} \rangle_P$$

$$\widehat{\mathbf{n}}\widehat{\Lambda} \rightarrow \mathbf{n}P - \mathbf{n}\frac{\partial P}{\partial \mathbf{n}}(\mathbf{I} \pm \mathbf{n})$$

$$\widehat{\Lambda}\widehat{\mathbf{n}} \rightarrow \mathbf{n}P - (\mathbf{I} \pm \mathbf{n})\frac{\partial P}{\partial \mathbf{n}}\mathbf{n} \,.$$

QUANTUM SIMULATION

INSOLUBLE QUANTUM EQUATIONS

$\longrightarrow$ COMPUTABLE STOCHASTIC EQUATIONS

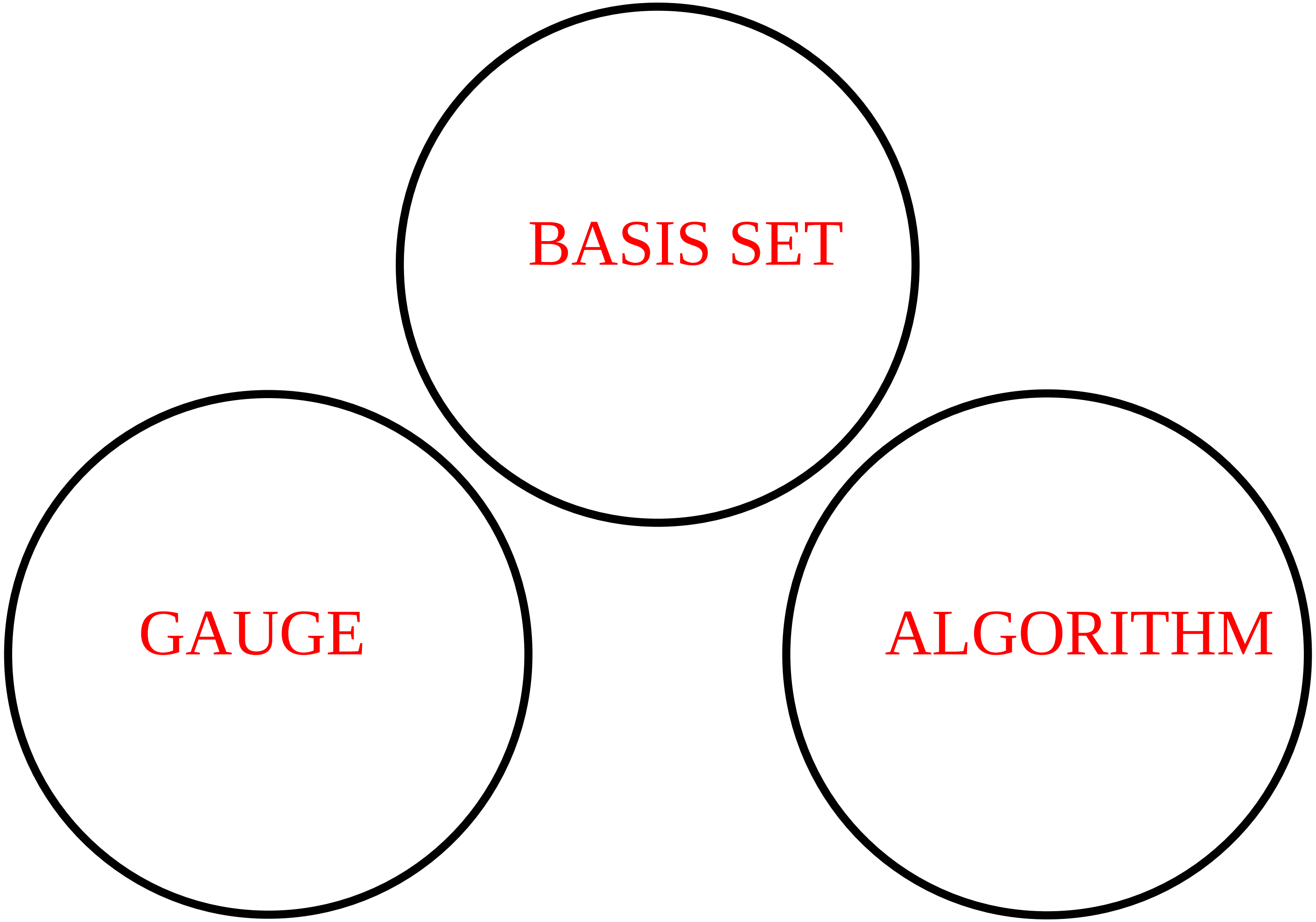
$$d\boldsymbol{\Omega}/\partial t = \boldsymbol{\Omega}\left[U + \mathbf{g}\cdot\zeta\right]$$

$$d\alpha/\partial t = \mathbf{A} + \mathbf{B}(\zeta - \mathbf{g})$$

SUCCESSES AND CHALLENGES

- ✔ Extension of Glauber, Sudarshan and Wigner
- ✔ No approximations - sampling error estimates possible
  - ✔ **Positive, nonsingular distributions**
  - ✔ **Reduces complexity enormously**
- ✘ Many trajectories to control sampling error
- ✘ **Stable trajectories to remove boundary-terms**

Different Strategies



APPLICATIONS

Unified method for three main types of problems studied:

- ✔ Canonical ensembles - thermal initial conditions
- ✔ Quantum dynamics - unitary nonlinear evolution
- ✔ Master equations - non-unitary evolution

- **Can be used for fermions AND bosons**

BOSONS

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

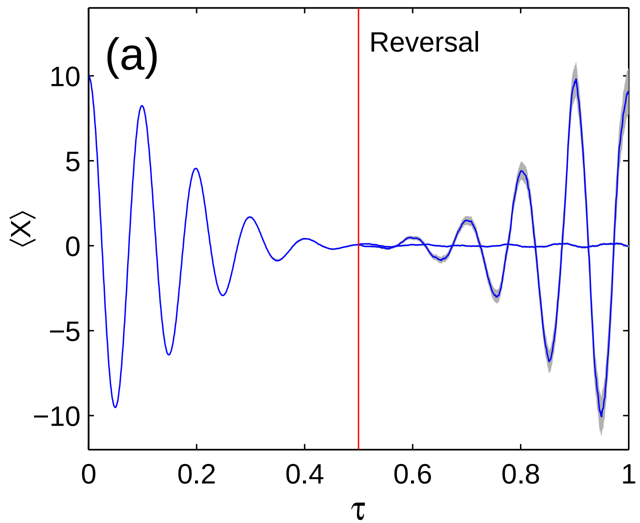
- $\widehat{H}(\mathbf{a},\mathbf{a}^{\dagger}) = \hbar\left[\sum\sum\omega_{ij}a_i^{\dagger}a_j + \sum : \widehat{n}_j^2 :\right]$.
- ω_{ij} - nonlocal coupling, includes chemical potential.
- Boson number: $\widehat{n}_i = a_i^{\dagger}a_i$.
- General approach also holds for quantum fields
- Simplest case: positive-P - $\widehat{\Lambda}(\overrightarrow{\lambda}) = \Omega\left|\alpha\right\rangle\left\langle\beta\right| / \left\langle\beta\right|\left.\alpha\right\rangle$.

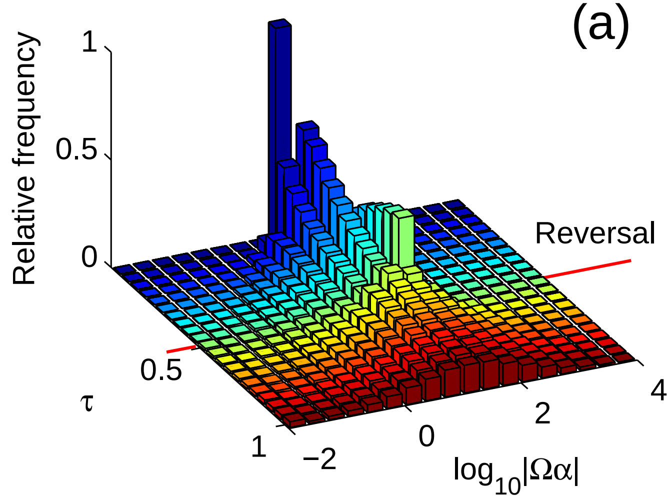
SINGLE-MODE TIME-EVOLUTION

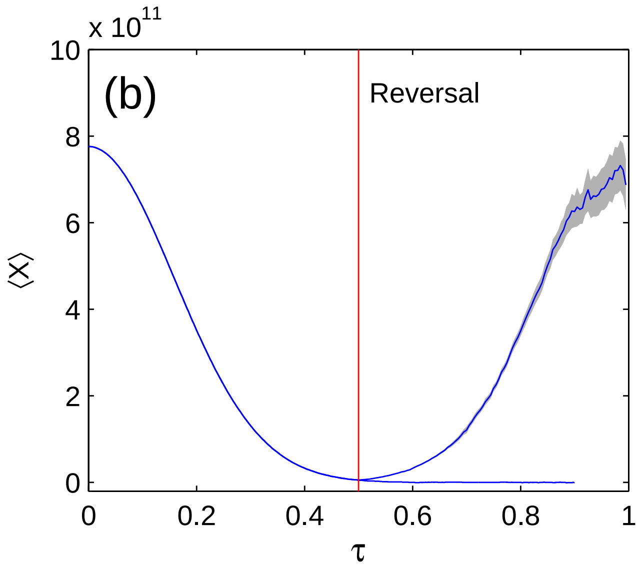
$$
\begin{aligned}
i\frac{d\alpha}{d\tau} &= \left[|\alpha\beta^*| + \omega + \sqrt{i}\zeta_1(\tau)\right]\alpha \\
i\frac{d\beta}{d\tau} &= \left[|\alpha\beta^*| + \omega + \sqrt{-i}\zeta_2(\tau)\right]\alpha^+ \\
\frac{d\Omega}{d\tau} &= \Omega g_i \zeta_i(\tau)
\end{aligned}
$$

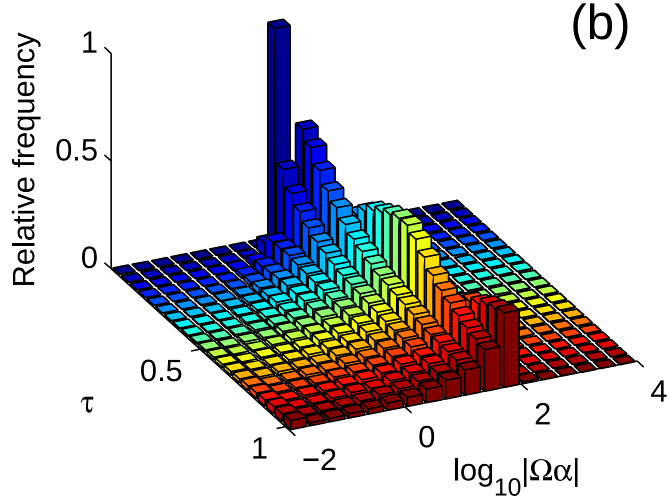
- Unitary evolution: 10^{23} bosons (PRL, 2005)!

Time-reversal test of unitary evolution







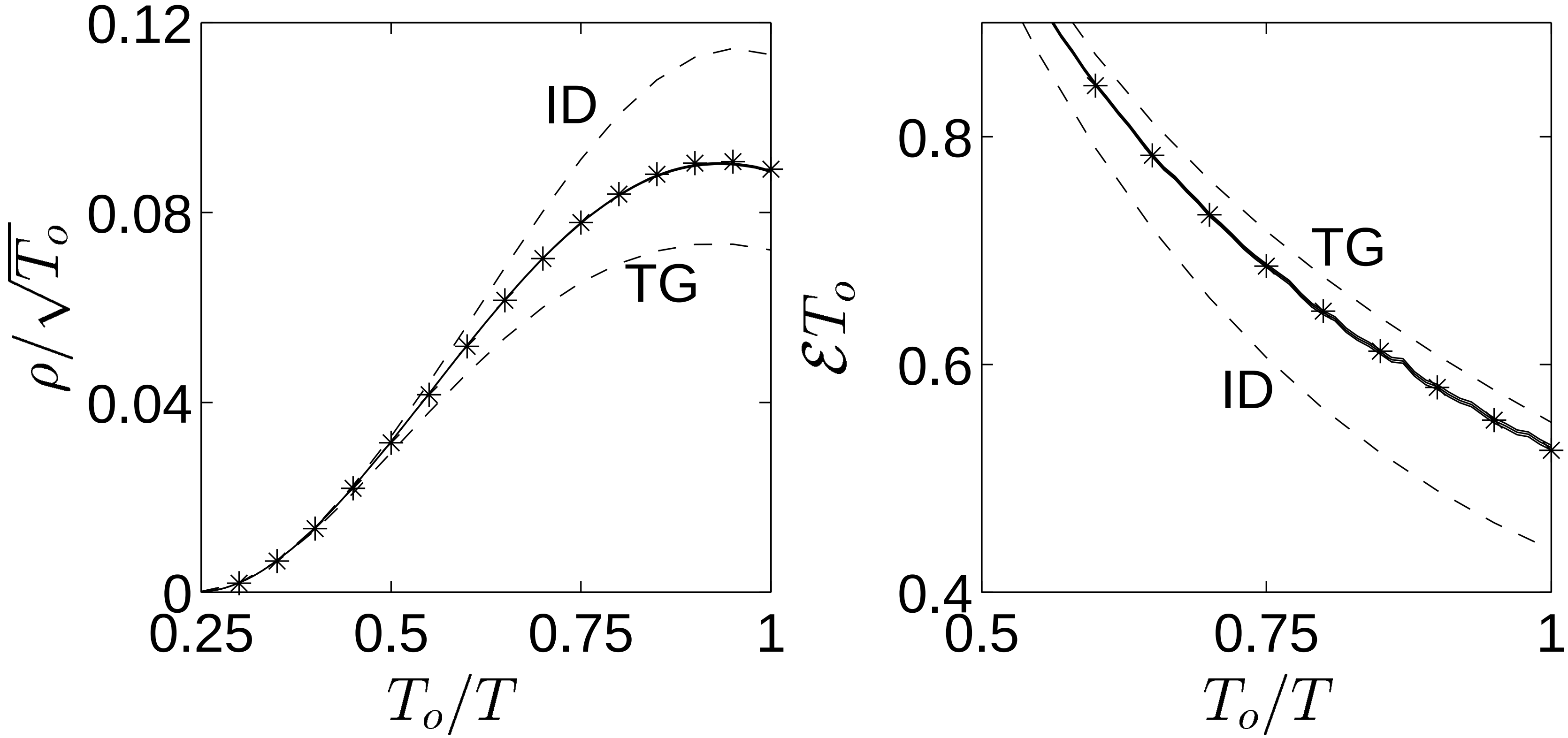


ONE-DIMENSION, FINITE TEMPERATURE

$$
\begin{aligned}
\frac{d\alpha}{d\tau} &= -\left[|\alpha\beta^*| + \omega - \nabla^2 + i\zeta_1(\tau)\right]\alpha \\
\frac{d\beta}{d\tau} &= -\left[|\alpha\beta^*| + \omega - \nabla^2 + i\zeta_2(\tau)\right]\beta \\
\frac{d\Omega}{d\tau} &= -H\Omega + gauge\,terms
\end{aligned}
$$

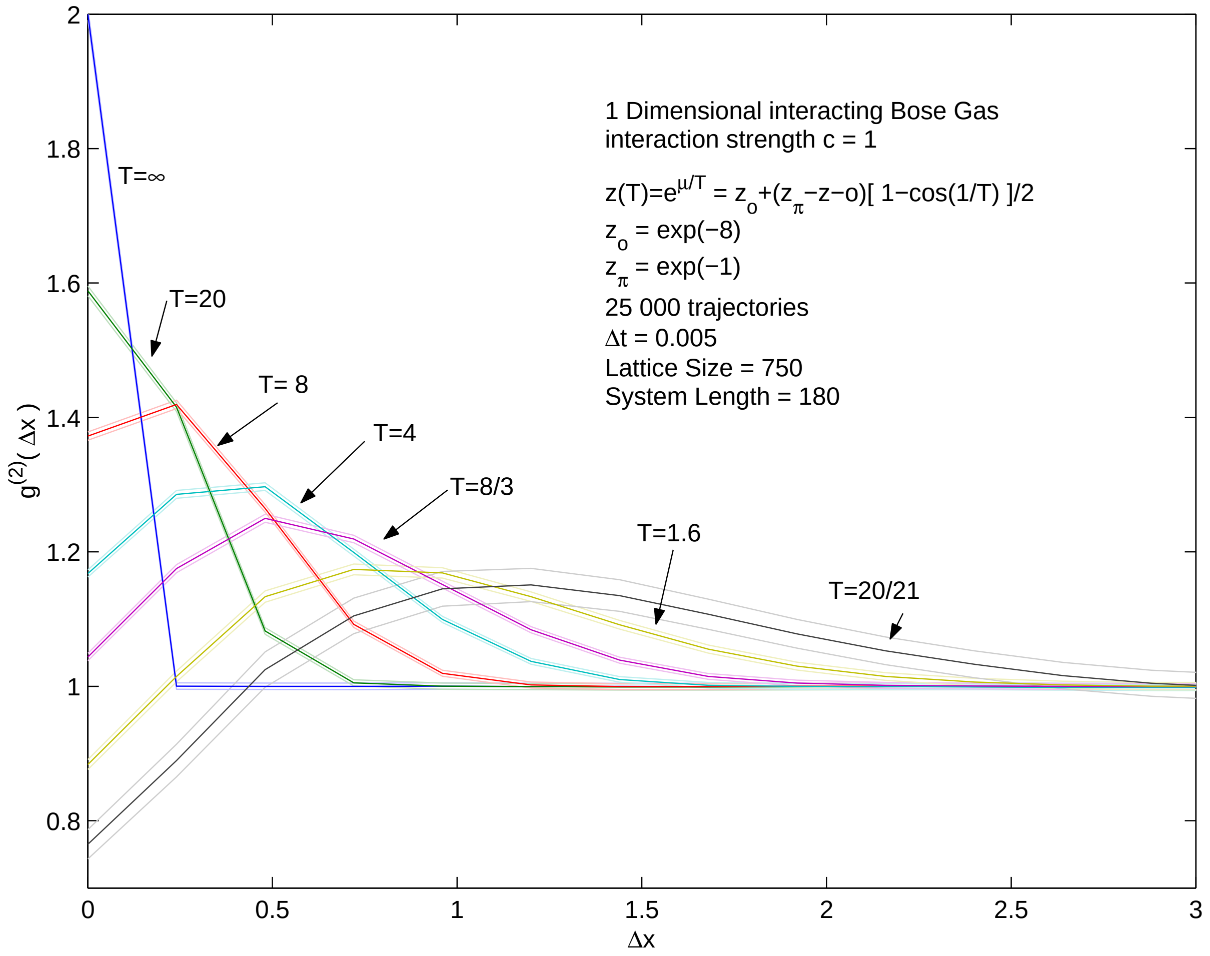
- $\alpha \longrightarrow$ Gross-Pitaevskii equation + quantum noise

1D +P Simulations vs exact results

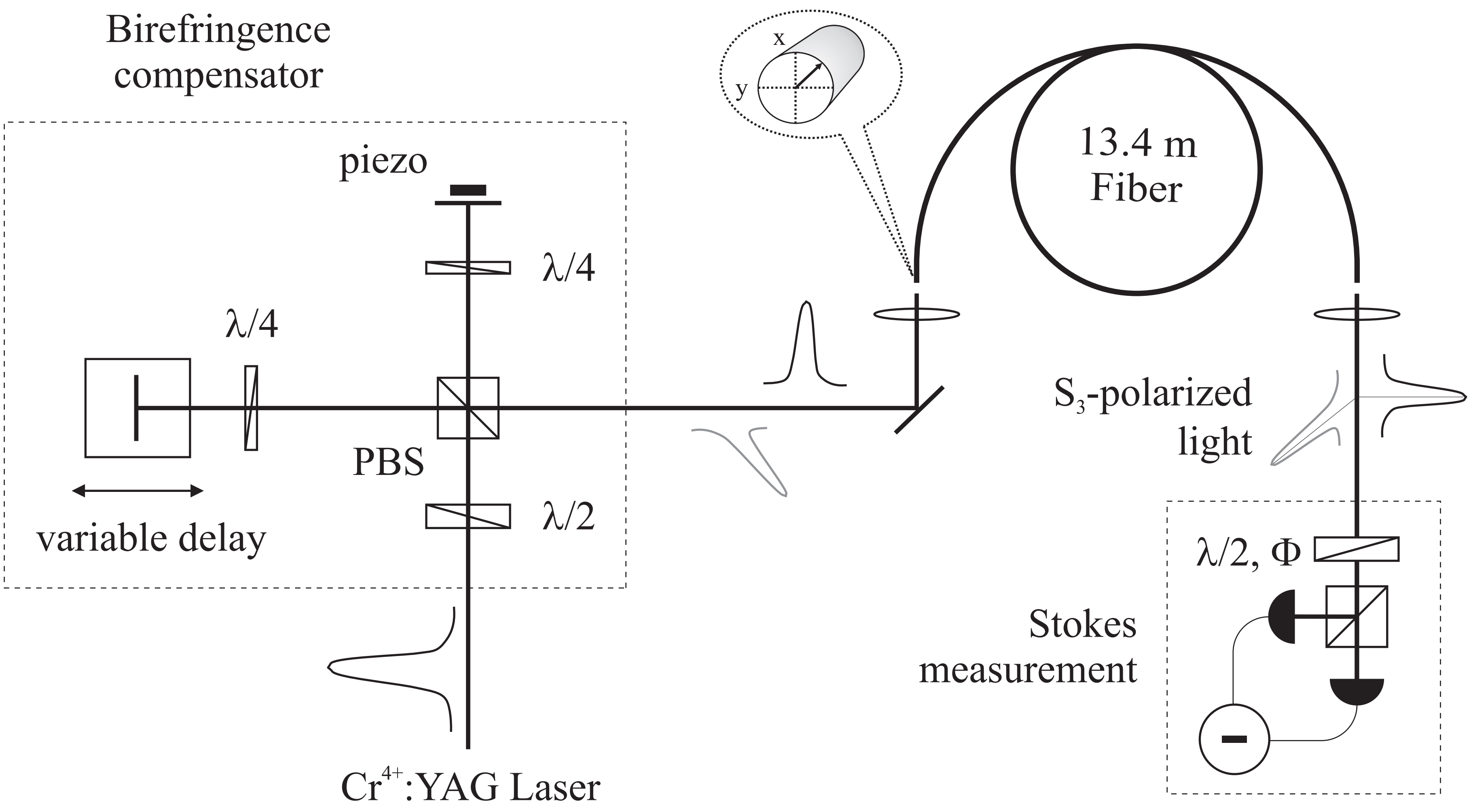


✔ Agreement with exact solutions (PRL, JAN, 2004)

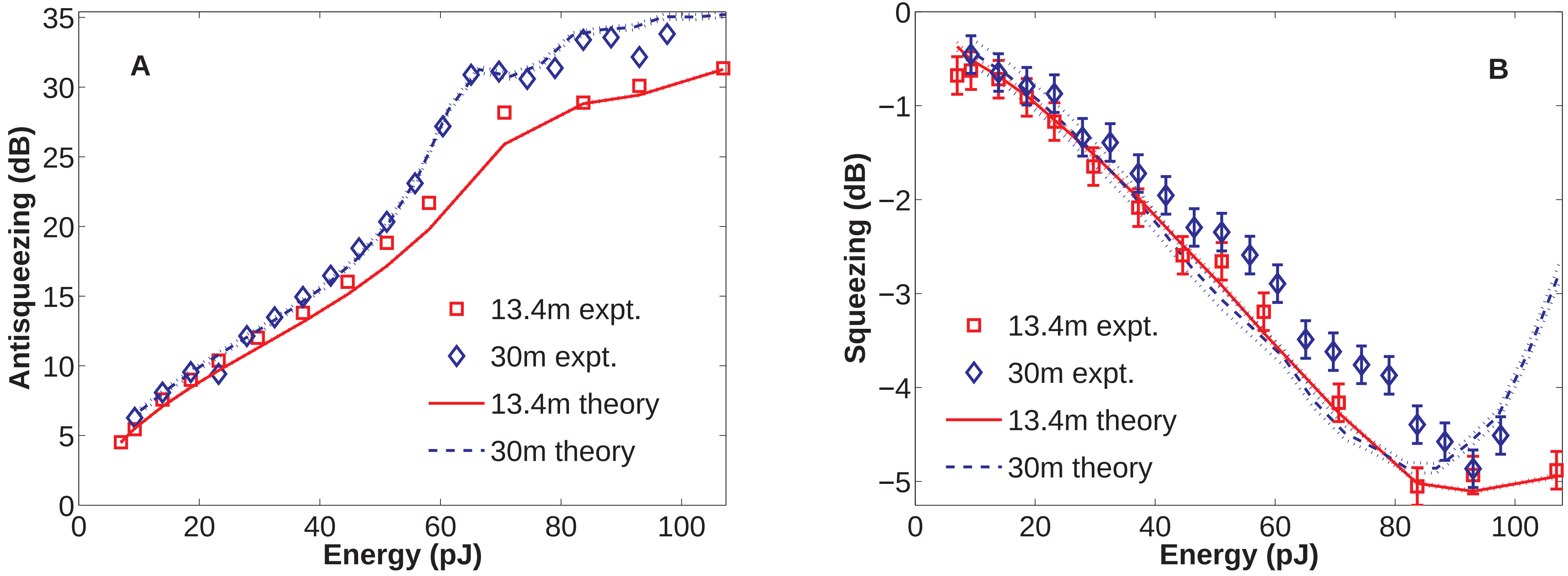
Spatial correlations: experiments underway



Optical fibre squeezing experiment

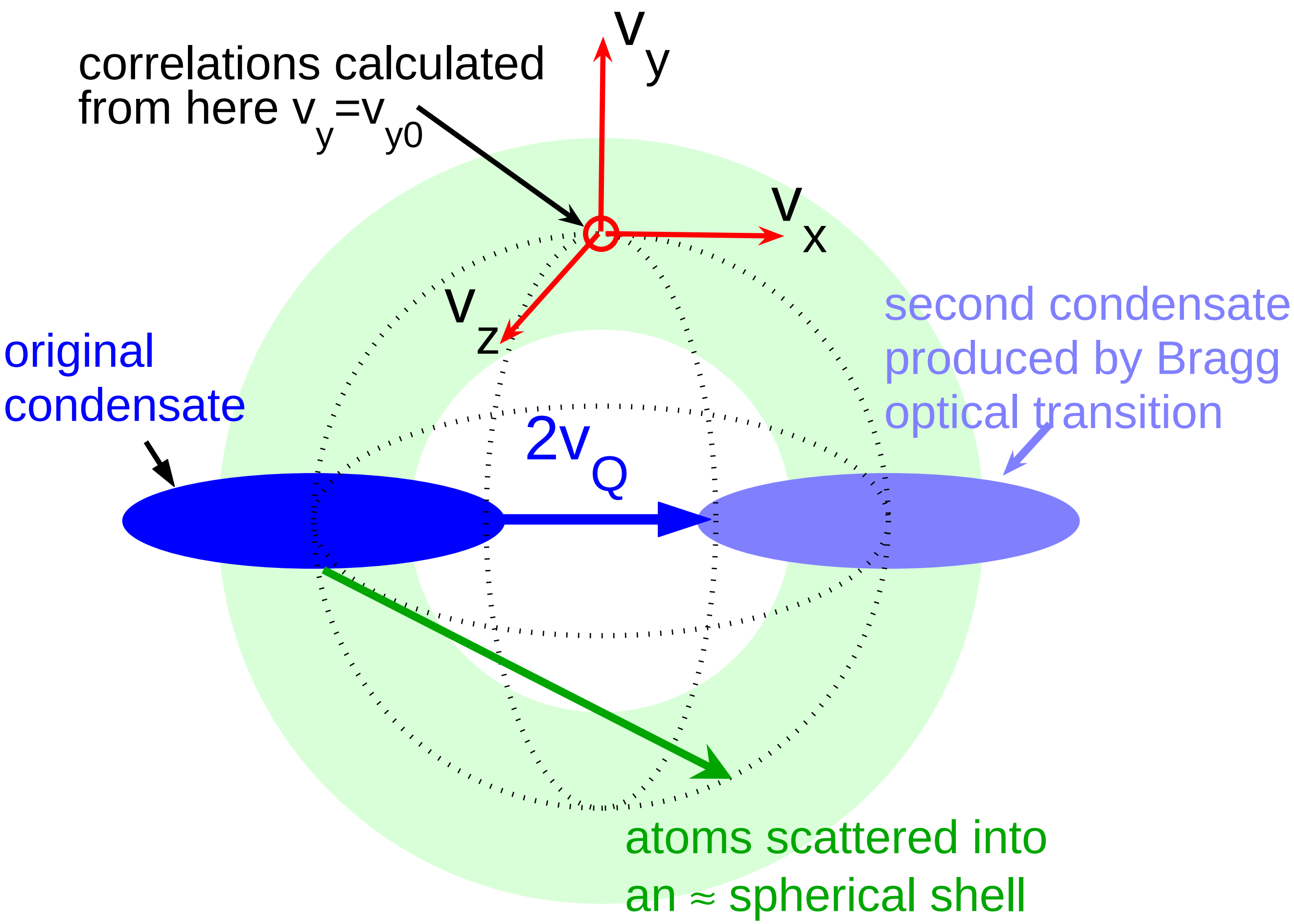


Wigner (or +P) simulation results

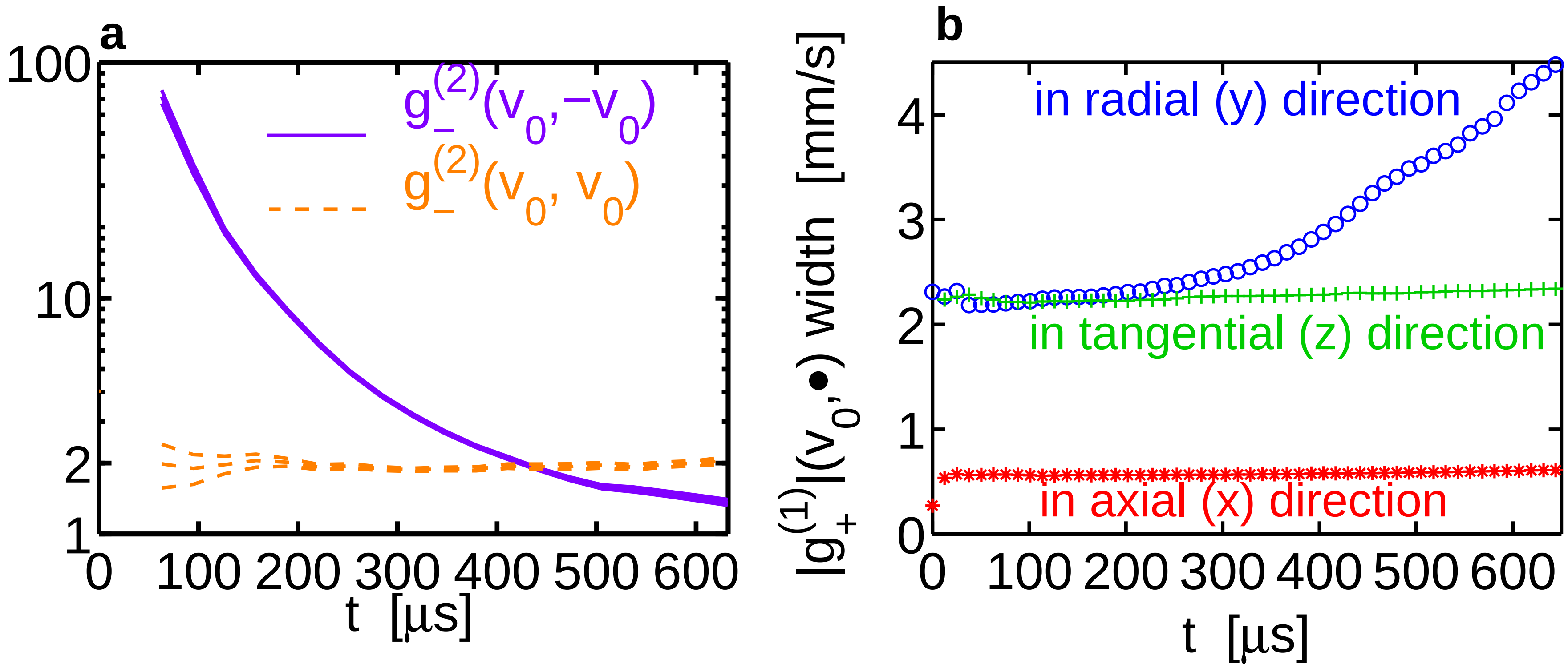


- antisqueezing and squeezing for $L = 13.4, 30m$ fibres
- parameters: $t_0 = 74\text{fs}$, $z_0 = 0.52\text{m}$, $\bar{n} = 2 \times 10^8$ photons

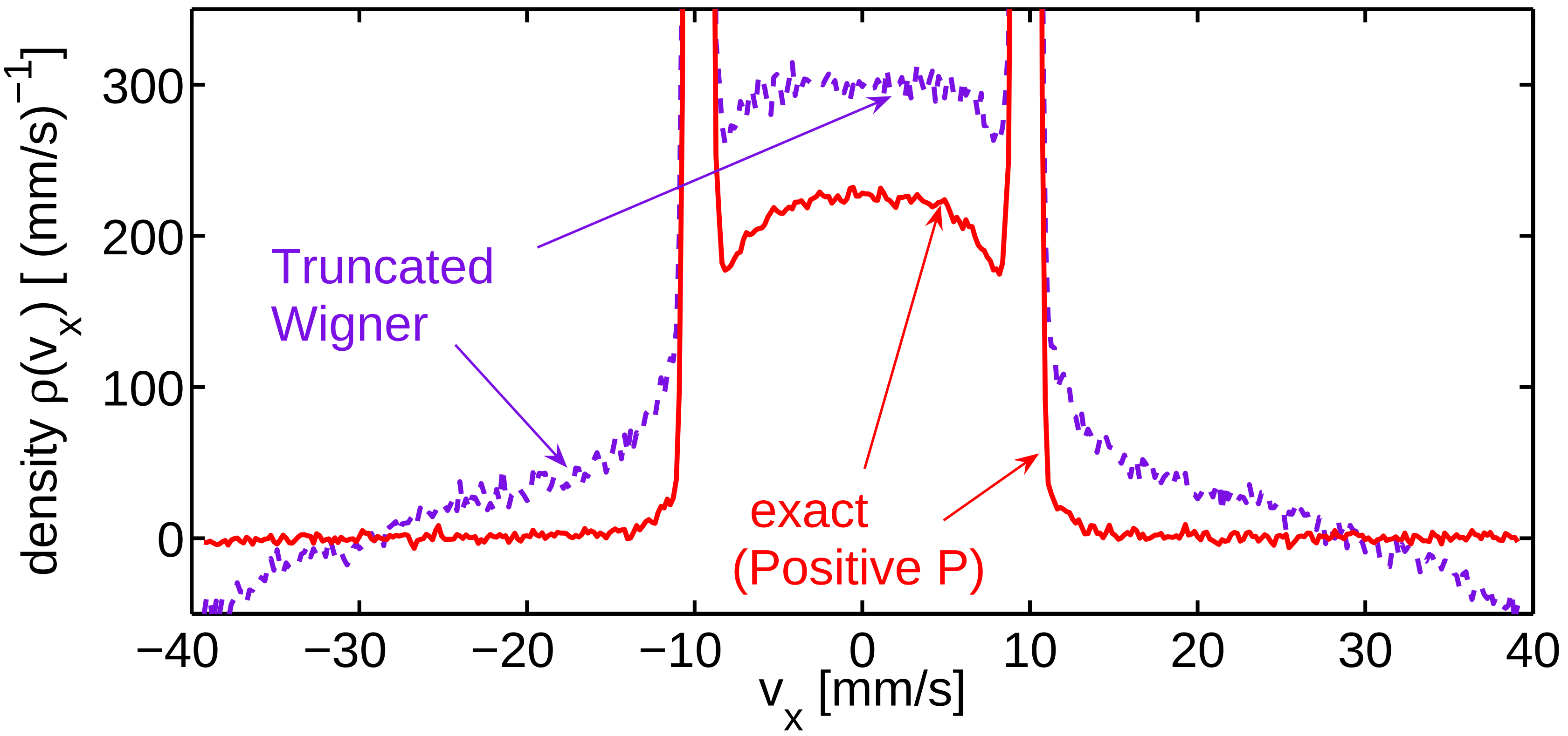
Four-wave mixing in a BEC collision



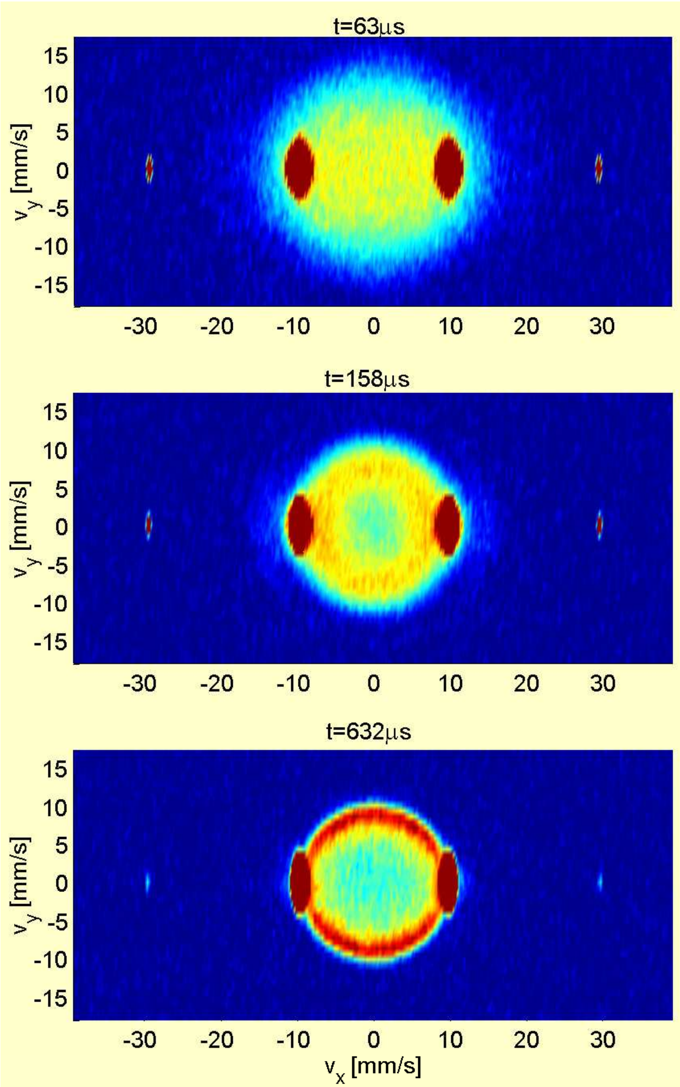
Correlations



Positive-P vs Wigner



Momentum-space snap-shots



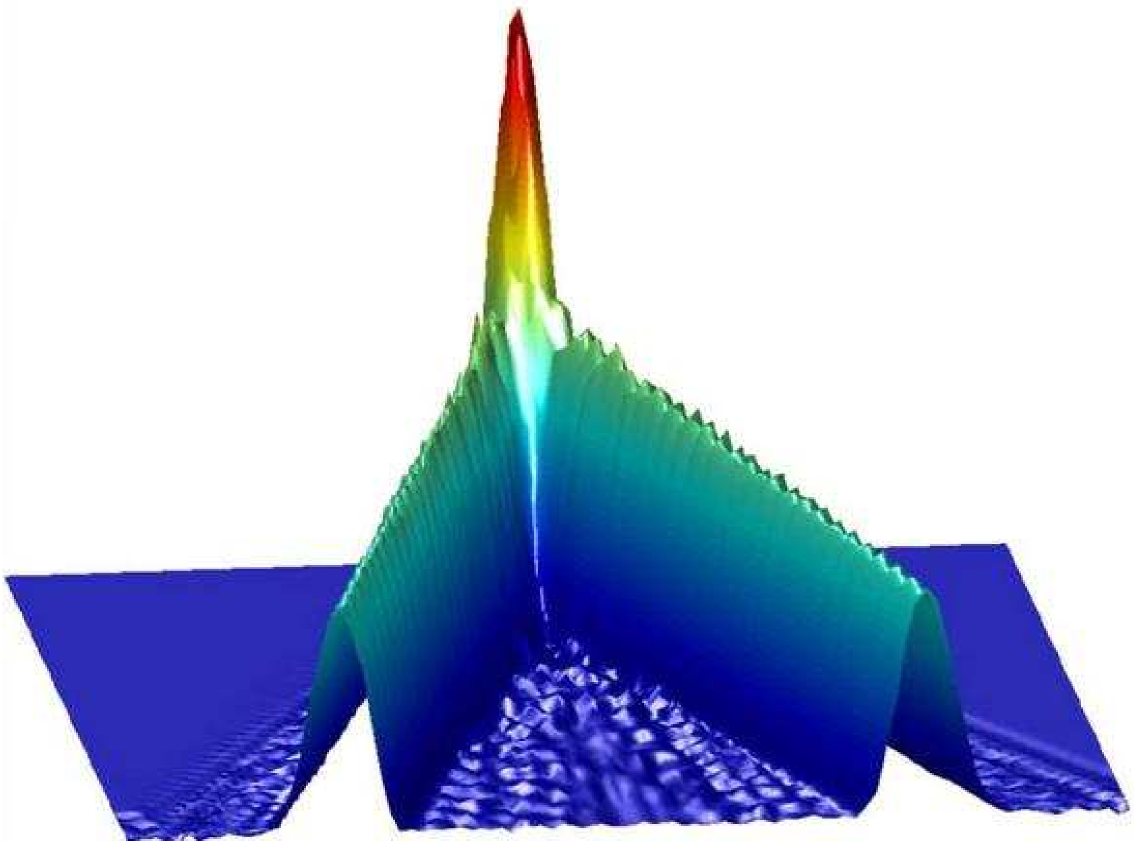
- Largest Hilbert space ever simulated
  - 10^5 atoms
  - 10^6 modes
  - 2×10^6 Q-bits
- First experiment: Ketterle, MIT
- Correlations: Westbrooke, Orsay
- **First-principles theory at UQ**

MOLECULAR DOWNCONVERSION

Hamiltonian: $\hat{H} = \hat{a}\widehat{b}_1^\dagger\widehat{b}_2^\dagger + h.c.$

- Can take place via Feshbach resonance or photodissociation
- Calculation in a 1D TRAP
  - **Quantum correlations and entanglement**
  - **Potential EPR experiment**

Molecular downconversion: NIST, Garching



FERMIONS

$$\widehat{H} = -\sum_{ij,\sigma} t_{ij} \widehat{a}^{\dagger}_{i,\sigma} \widehat{a}_{j,\sigma} + U \sum_{j} : \widehat{n}_{j,j,\downarrow} \widehat{n}_{j,j,\uparrow} :$$

- Simplest model of an interacting Fermi gas on a lattice
- Describes ultracold gas in an optical lattice: experiments at ETH, Zurich
  - **Weak-coupling limit $\longrightarrow$ BCS transitions**
  - **Relevance to high-T_c superconductors**

QMC sign problem

- Traditional fermionic Quantum Monte Carlo (QMC) suffers from sign problems:

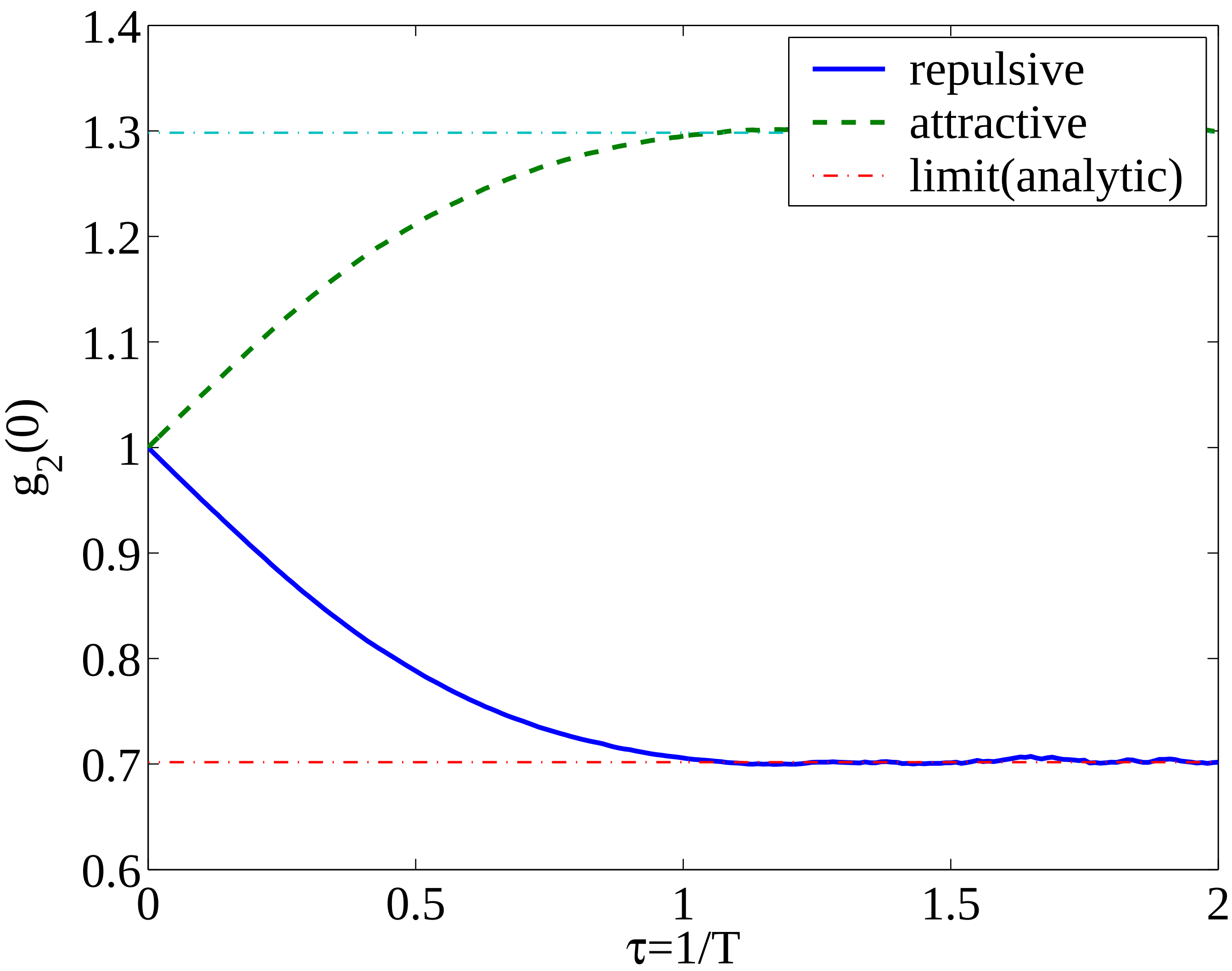
$$\langle A \rangle \sim \frac{\langle sA \rangle}{\langle s \rangle}$$

- sign problem increases with:
  - dimension, lattice size, interaction strength

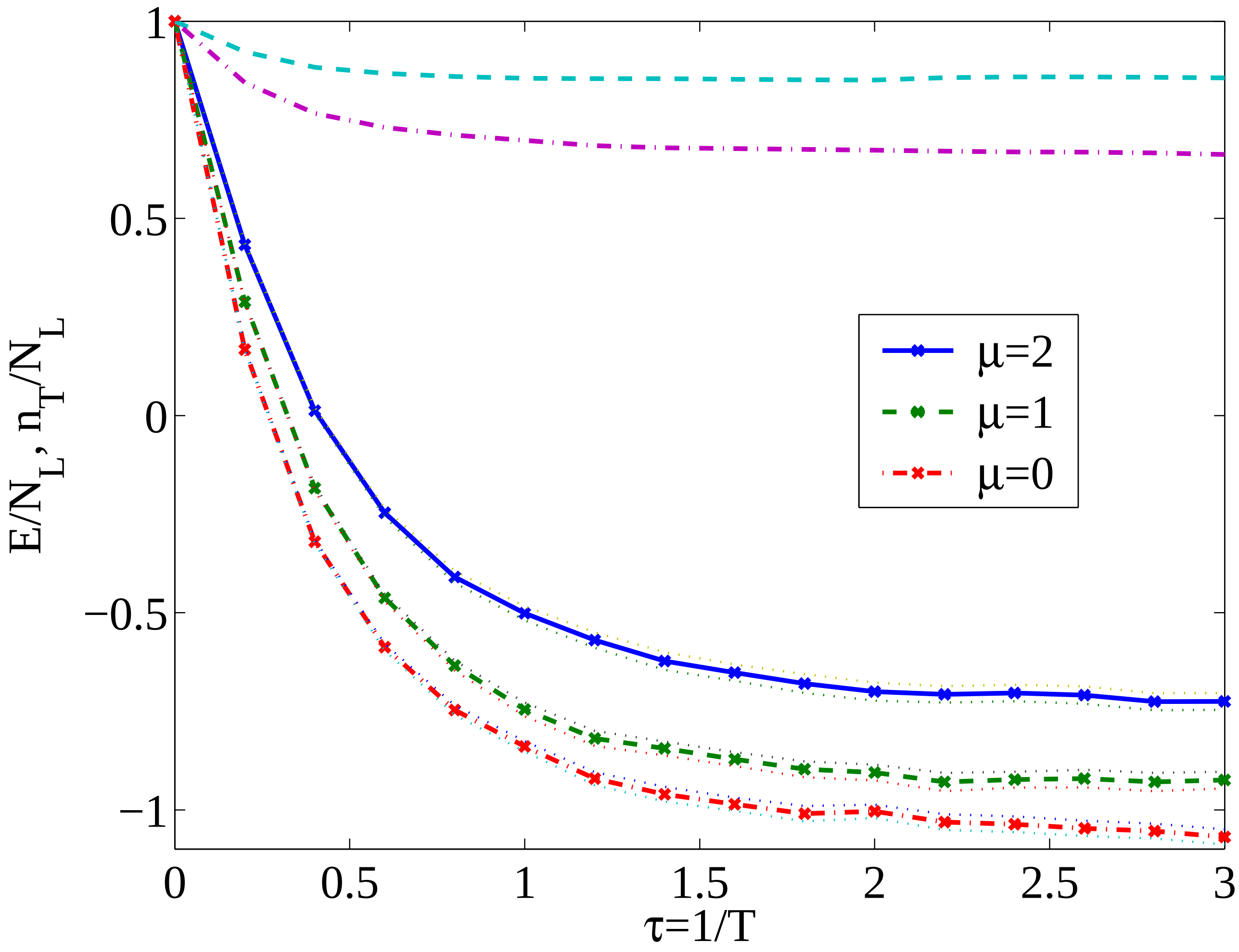
Finite-temperature phase-space equations

- Positive weights: $d\Omega/d\tau = -\Omega H(\mathbf{n}_1, \mathbf{n}_{-1})$
- Paths: $d\mathbf{n}_\sigma/d\tau = \frac{1}{2}\left\{(\mathbf{I}-\mathbf{n}_\sigma)\,T^{(1)}_\sigma \mathbf{n}_\sigma + \mathbf{n}_\sigma T^{(2)}_\sigma(\mathbf{I}-\mathbf{n}_\sigma)\right\}$.
- T-matrix: $T^{(r)}_{i,j,\sigma} = t_{ij} - \delta_{i,j}\left\{U(n_{j,j,-\sigma} - n_{j,j,\sigma} + \frac{1}{2}) - \mu + \sigma\xi^{(r)}_j\right\}$.
- Noises: $\left\langle \xi^{(r)}_j(\tau)\,\xi^{(r')}_{j'}(\tau')\right\rangle = 2U\delta(\tau-\tau')\delta_{j,j'}\delta_{r,r'}$.

1D Lattice - 100 sites vs: exact result



16x16 2D Lattice



No sign problem!

Genetic mutations

- **Genetic evolution of a population is also complex:**
- Suppose we consider 500,000 viruses (eg, HIV infection)
- Consider 20 sites in a genome, with two configurations
- Each virus can be in any of a million genotypes!
- Number of viral ecosystem states: $N_s > 10^{100,000}$!!

XMDS

- Generate C++ code from a short XML script
- Provides semantic (meaningful) program
- Up to 30 times faster than Matlab
- Ten times less code, less bugs
- Automatic message-passing on clusters
- XMDS-II - with user libraries - under development

SUMMARY

- Gaussian quantum phase-space: extends coherent-state methods
- Representations for bosons **and** fermions
- Up to 3D simulations, up to 10^{23} particles, 10^{6} modes
- **EQUIVALENT TO ~ MILLION QUBITS**
- Other complex systems - genetics, biochemistry?
- Many interesting challenges: new computational physics

ACQAO Theory @ University of Queensland