First-principles simulations of 1D Bose gasses using stochastic gauges

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Many-mode Quantum Simulations

- Recent experiments are probing the 1D Bose Gas.[Orzeł *et. al.* 2001; Görlitz *et. al.* 2001].

- The smaller number of relevant modes in 1D allows better chance of a first-principles simulation, rather than just mean-field or perturbation theory.

- Many properties of 1D bose gas are unknown. In fact, for thermal interacting bosons, *only* exact result is density and total energy (with no trap). [Yang&Yang 1969].

- Many-body simulations are notoriously difficult because of the rapid growth of Hilbert space with number of bodies.

- "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*)

Efficiency of Numerical Methods

For M modes, E significant eigenstates per mode.

Method	**Number of Complex Equations**	**Stochastic?**
Direct Solution of Denity Matrix	$(E^M)^2$	No
Quantum Trajectories	E^M	Yes
Positive P representation	$2M$	Yes
Hermitian P representation	$2M+1$	Yes

The stochastic methods require averaging over a number of realisations to obtain physical quantities.

The P distribution methods are clearly the only practical methods for many modes.

Hermitian P representation

- Expand density matrix in off-diagonal coherent-state projection operators with a quantum phase

$$\hat{\rho} = \int P(\vec{\alpha},\vec{\beta},\Omega)\frac{|\vec{\alpha}><\vec{\beta}|^*}{<\vec{\beta}^*|\vec{\alpha}>}e^{\Omega}\; d^{2M}\vec{\alpha}\; d^{2M}\vec{\beta}\; d^2\Omega$$

$$+ \text{ hermitian conjugate}$$

- $P(\vec{\alpha},\vec{\beta},\Omega)$ is a positive, normalised distribution function which exists for all density matrices.

- Master equation for $\hat{\rho}$ can be made equivalent to a Fokker-Planck pde. for P, and subsequently to a system of stochastic equations for the variables $\vec{\alpha},\vec{\beta},\Omega$.

- Avoids the technical difficulties of positive P representations at low mode occupation.

Dynamics

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right] + \hat{\mathcal{L}}\{\hat{\rho}\}$$

$\hat{\mathcal{L}}$: Losses

Thermodynamics

$$\frac{\partial \hat{\rho}_u}{\partial \tau} = -\frac{1}{2}\left[\frac{\hat{H}}{\hbar} - \mu(\tau)\hat{N}, \hat{\rho}_u\right]_+$$

$$\tau = \hbar/(k_B T)$$

- $\hat{\rho}_u$ is the equilibrium state at temperature T.
- P representation is equivalent to density matrix, so can easily transfer from time-dependent to temperature-dependent calculations.

Quantum model of a BEC

Neutral atoms in $d = 1, 2,$or3 dimensions:

$$\hat{H} = \int d^d\mathbf{x} \Big[$$

$$\frac{\hbar^2}{2m}\nabla\hat{\Psi}^\dagger(\mathbf{x})\nabla\hat{\Psi}(\mathbf{x})$$

Kinetic Energy, mass m

$$+V(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})$$

Trapping Potential $V(\mathbf{x})$

$$+\hat{\Psi}^\dagger(\mathbf{x})\hat{R}(\mathbf{x})+\hat{\Psi}(\mathbf{x})\hat{R}^\dagger(\mathbf{x})$$

Localized Loss at rate $\propto$Tr$[R(\mathbf{x})]$

$$+\frac{1}{2}\int d^d\mathbf{y}U(\mathbf{x}-\mathbf{y})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{y})\hat{\Psi}(\mathbf{y})\hat{\Psi}(\mathbf{x})$$

Boson-Boson Interaction $U(\mathbf{x}-\mathbf{y})$.

$$\Big]$$

Stochastic equations

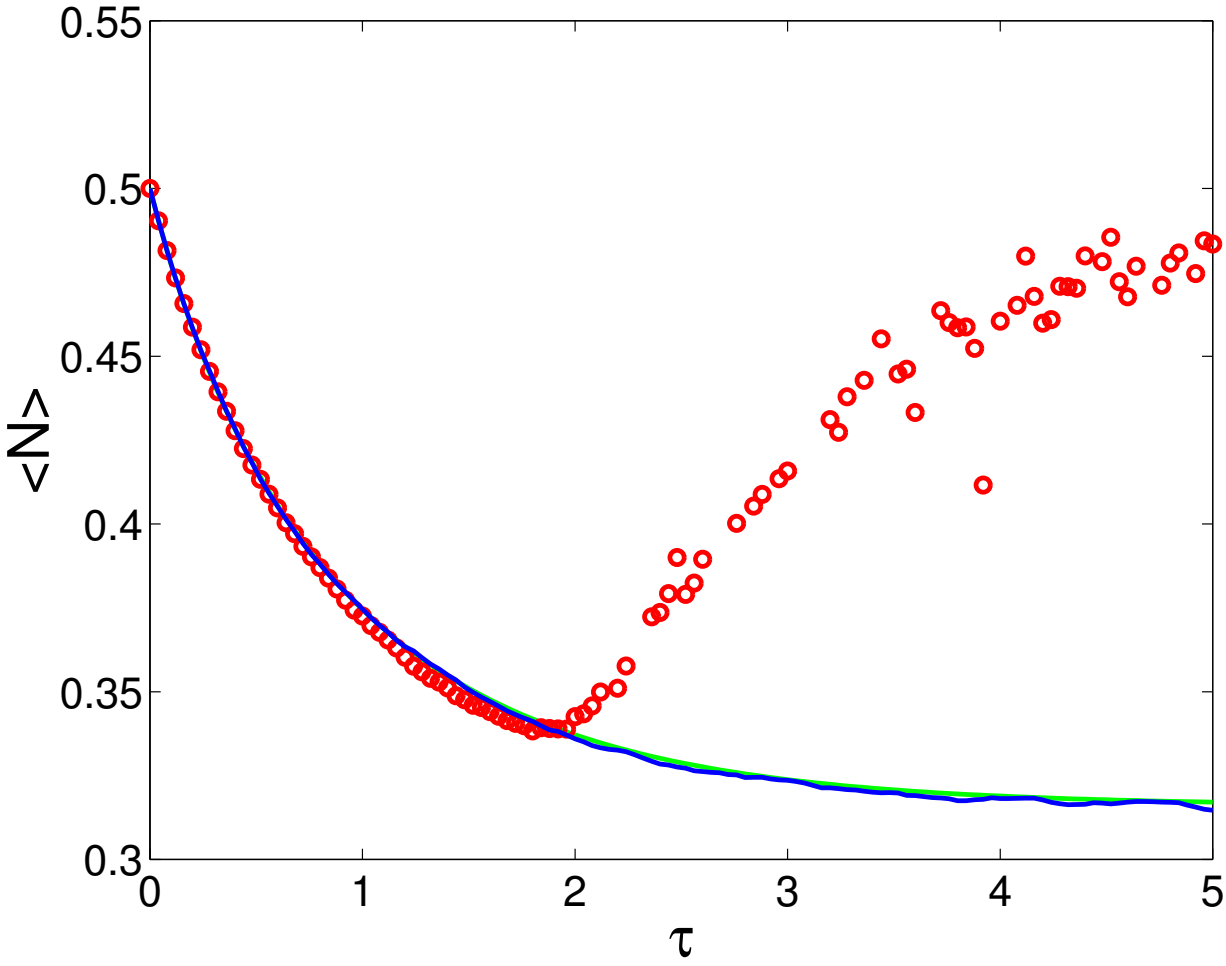
- Full quantum equations like the Gross-Pitaevskii (GP) mean-field equations, with appropriate noise terms added.

- Having a quantum phase in the basis operators of the distribution allows us to insert **arbitrary functions** (STOCHASTIC GAUGES) which we can fiddle to make the equations behave nicely, without changing the observeables.

- Previous difficulties with positive P simulations at low mode occupations fixed by judicious introduction of stochastic gauges.

1 mode: Zero chemical potential

$$\mu = 0$$

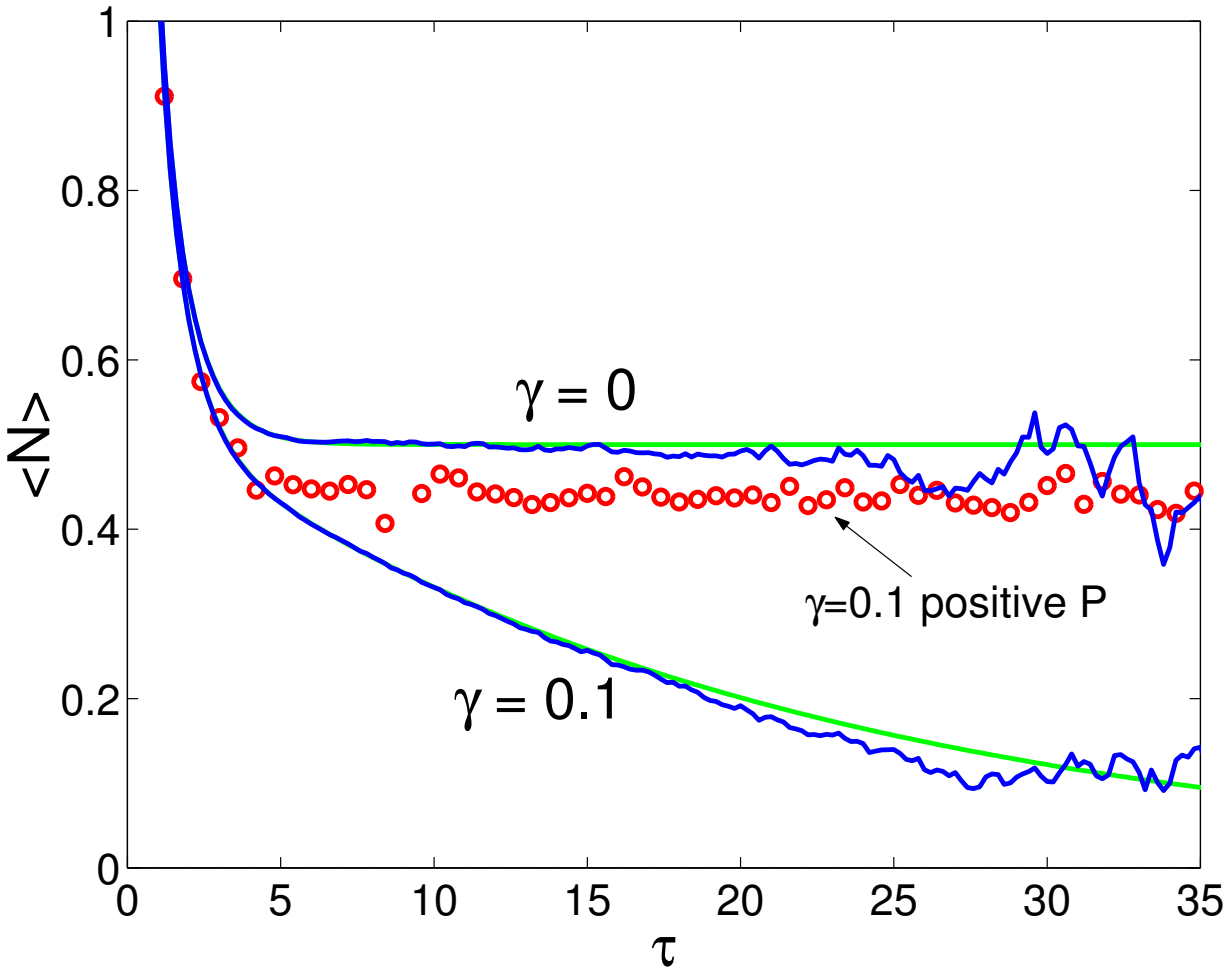


Circles: positive P simulation

Blue line: hermitian P gauge simulation.

Green line: exact calculation (truncated number-state basis).

1 mode: Non-zero chemical potential $\mu = -\gamma U$.



Circles: positive P simulation, $\gamma = 0.1$;

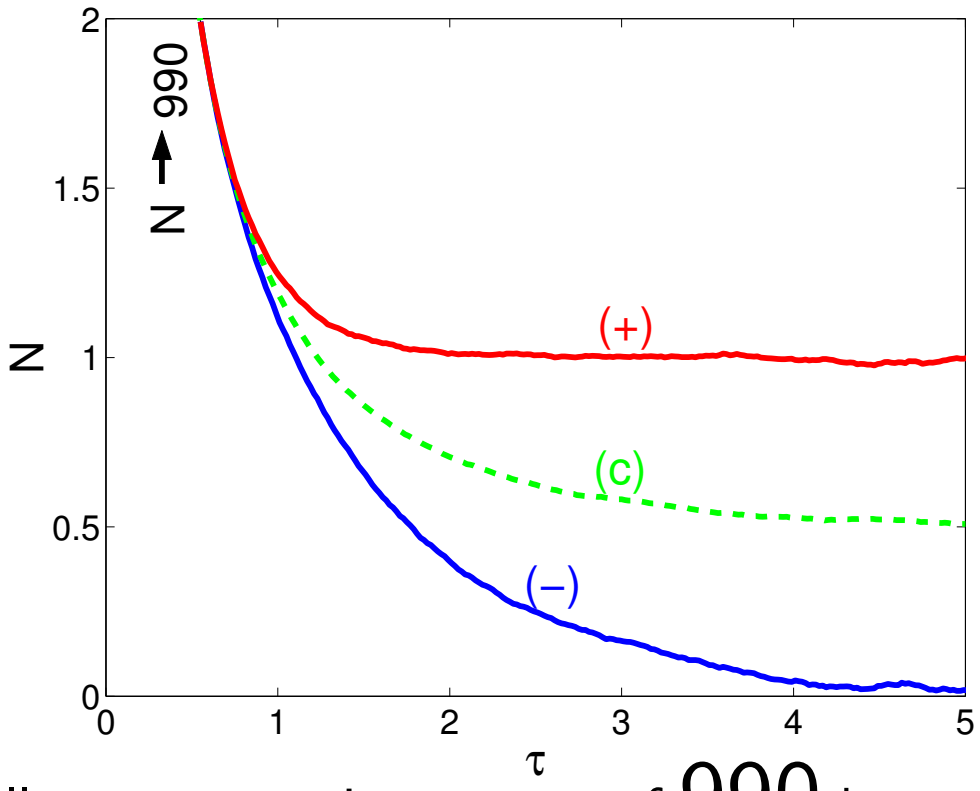
Blue line: hermitian P gauge simulations;

Green line: exact calculations (truncated number-state basis).

1 mode: Cat state evolution

Despite the noise, the Hermitian P simulation preserves extremely fragile quantum features such as the parity of a mesoscopic "cat" state.

$$|\psi(0)>=\frac{1}{\sqrt{2}}[\ |\ \alpha_o> \pm |-\alpha_o>\ ]$$



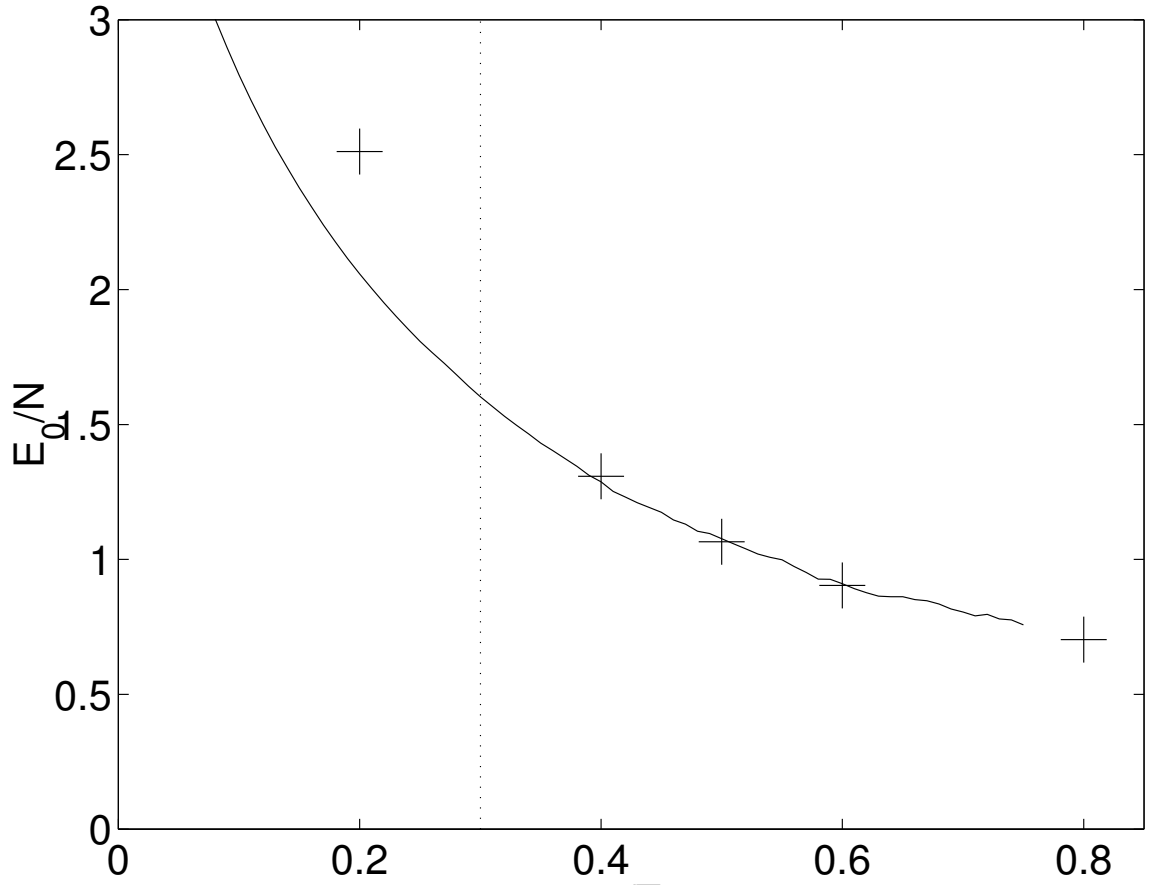
Initially, state contains average of 990 bosons:

Red: Odd "cat" - only odd numbers of photons

Blue: Even "cat" - only even numbers of photons

Green: Coherent state

Preliminary 1D calculations



1D Bose gas energy per particle. Variables scaled.

Number of particles in simulation around 100.

'+' – exact results from Yang&Yang solution.

solid line – stochastic gauge simulation.

Energy for $1/T < 0.3$ is known to be
under-estimated due to a fixed momentum cutoff.

Summary

- Can make many-body simulations scale linearly with number of modes.

- Solved the technical problems inherent at low mode occupations.

- Dynamical calculations of evaporative cooling implemented [See Poster by Tim Vaughan].

- BEC Thermodynamics? - work in progress.