

A Hybrid Phase-Space Representation for BEC Simulations

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The Hybrid Scheme

Problem:

- ★ quantum mechanics of a Bose-Einstein condensate
- ★ atoms in a trap, scattering from each other via a pairwise s-wave interaction
- ★ prediction of correlation function $g^{(2)}$

Method (Phase-space method, stochastic simulation):

- ★ **Use Wigner for highly occupied modes**
- ★ **Use Positive P for lightly occupied modes**

This representation (of a density matrix) is included in the class of **Gaussian representations** (Corney and Drummond)

Stochastic Phase-Space Methods

From the evolution of the density matrix

$$i \frac{\partial \rho}{\partial t} = [H, \rho]$$

we derive the evolution of a “quasiprobability”, a function on coherent state phase space

$$\frac{\partial Q(\vec{\alpha})}{\partial t} = - \sum_i V_i(\vec{\alpha}) \frac{\partial Q}{\partial \alpha_i} + \frac{1}{2} \sum_{ij} D_{ij}(\vec{\alpha}) \frac{\partial}{\partial \alpha_i} \frac{\partial}{\partial \alpha_j} Q(\vec{\alpha}) + \dots$$

Stochastic Phase-Space Methods (cont.)

Calculation of expectation values:

Wigner:
$$\int d^2\alpha W(\alpha) |\alpha|^2 = \langle a^\dagger a \rangle + \frac{1}{2}$$

Positive P:
$$\int \int d^2\alpha d^2\beta P(\alpha, \beta^*) \beta^* \alpha = \langle a^\dagger a \rangle$$

Stochastic differential equations to model the evolution of $Q(\vec{\alpha})$:

- ★ finite sample of trajectories governed by **drift** and **diffusion**
- ★ ensemble averages of trajectory variables estimate the desired integrals

To be able to do this:

- ★ must have **derivatives** no higher than **2nd order**
- ★ must have a **diffusion matrix** that is **positive semidefinite** (all eigenvalues ≥ 0)

Features of The Wigner Representation

- ☆ The quasiprobability, $W(\alpha)$, is **not** guaranteed to be **positive** everywhere
- ☆ However, it is positive for a **coherent state** initial condition
- ☆ **TRUNCATION** of derivatives higher than **2nd order**
 - May be justified for highly occupied modes
 - What starts positive stays positive, if diffusion matrix is **positive semidefinite**
 - Therefore stochastic simulation is possible
- ☆ **Truncation removes physics**: find disagreements with other methods and with experiment

Features of the Positive P Representation

- ★ Implicit definition of quasiprobability, $P(\alpha, \beta^*)$: **not unique**
- ★ Can always choose **initial** $P(\alpha, \beta^*)$ **everywhere positive**
- ★ With Hamiltonians of interest, only get **2nd order derivatives**
- ★ Diffusion matrices are always **positive semidefinite**
- ★ Therefore a stochastic simulation is possible
- ★ Sampling error may become large after a short simulation time
 - due to modes that develop wide distributions in phase space

Expectations for the Hybrid Method

PRO: Should be like using the Wigner representation without the discrepancies associated with lightly occupied modes

PRO: May be able to identify modes that spread widely in phase space, treat them with Wigner

CON: Ultraviolet divergence problem of 3D simulations will occur here too

★ worst for Wigner representation: initial noise

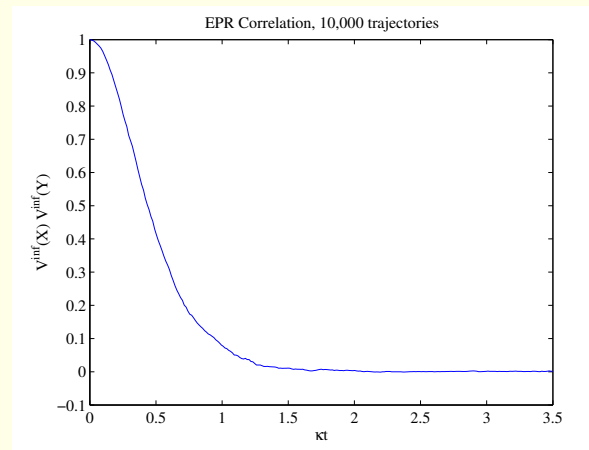
Preliminary Results

★ Ketterle four-wave mixing experiment in an optical lattice

★ Three different modes: $2a \rightarrow b + c$

$$H = \omega_a a^\dagger a + \omega_b b^\dagger b + \omega_c c^\dagger c + i\chi \{ b^\dagger c^\dagger a^2 - (a^\dagger)^2 bc \}$$

★ Agreement between Wigner, Positive P and Hybrid (for short simulation times)



Possible Experiments to be Simulated

Individual particle detection and colliding BECs

- ★ Aspect metastable He
- ★ ANU metastable He
- ★ Ketterle four-wave mixing: full 3D simulation

Conclusions

- ★ A new phase-space representation
- ★ Possible ways to improve on Wigner and Positive P methods
- ★ Seeking a general method for a wide range of BEC calculations.