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

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

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 for highly occupied modes - eg, a condensed mode

PRO: Treats nearly unoccupied modes using a normally ordered +P method: so there are no ultraviolet divergences in `virtual' particles

CON: Ultraviolet divergence problems in time-evolution of 3D simulations?

✯ OPEN QUESTION: NEED TO TRY THIS!

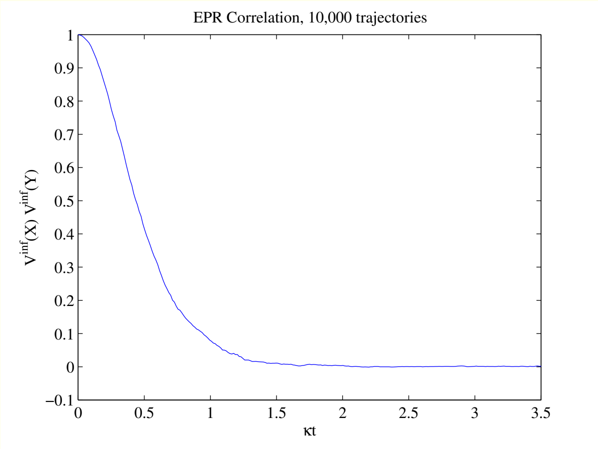
Preliminary Results

✯ Ketterle four-wave mixing experiment in an optical lattice

✯ Three different modes: $2a \longrightarrow b + c$

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

✯ 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.