Gaussian Phase-Space Representations III

Vssup Lectures 2012

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Outline

What is the BEC Hamiltonian?

What about the quantum fields with hats?

Recall from the BEC lectures $\widehat{\Psi}_i$ is a quantum field of spin-index i:

$$\left[\widehat{\Psi}_i(\mathsf{x}), \widehat{\Psi}_i^\dagger(\mathsf{x}')\right]_\pm = \delta_{ij}\delta^D(\mathsf{x}-\mathsf{x}')$$

In second quantization the quantum Hamiltonian is

$$\begin{aligned}\widehat{H} &= \sum_i \int d^D\mathsf{x}\left\{\frac{\hbar^2}{2m}\nabla\widehat{\Psi}_i^\dagger(\mathsf{x})\cdot\nabla\widehat{\Psi}_i(\mathsf{x}) + V_i(\mathsf{x})\widehat{\Psi}_i^\dagger(\mathsf{x})\widehat{\Psi}_i(\mathsf{x})\right\} \\ &+ \sum_{ij}\frac{U_{ij}}{2}\int d^D\mathsf{x}\,\widehat{\Psi}_i^\dagger(\mathsf{x})\widehat{\Psi}_j^\dagger(\mathsf{x})\widehat{\Psi}_j(\mathsf{x})\widehat{\Psi}_i(\mathsf{x})\,.\end{aligned}$$

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What are the parameters?

This describes a dilute gas at low enough temperatures,

- $\langle \widehat{\Psi}_i^\dagger(\mathbf{x})\widehat{\Psi}_i(\mathbf{x})\rangle$ is the spin i atomic density,
- m is the atomic mass,
- V_i is the atomic trapping potential & Zeeman shift
- U_{ij} is related to the S-wave scattering length in three dimensions by:

$$U_{ij} = \frac{4\pi\hbar^2 a_{ij}}{m}.$$

- Here we implicitly assume a momentum cutoff $k_c << 1/a$

Local Mode Operators

Assume that the mode operators are localized on a lattice

Spin and position indices $= \{s_k, \mathbf{r}_k\}$ with lattice volume ΔV:

$$\hat{a}_i = \sqrt{\Delta V}\widehat{\Psi}_{s_k \mathbf{r}_k}$$

In the case of bosonic (fermionic) fields, the commutators (anticommutators) are defined as:

$$\left\{\hat{a}_i, \hat{a}_j^\dagger\right\}_\pm = \delta_{ij}$$

The Hamiltonian is exact for a large number of sites:

$$\widehat{H}(\hat{a}^\dagger, \hat{a}) \approx \hbar \sum_{ij} \left[\omega_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\chi_{ij} : \widehat{n}_i \widehat{n}_j :\right].$$

Losses and damping?

Damping can be treated using a master equation

- The density matrix $\hat{\rho}$ evolves as:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}\left[\hat{H},\hat{\rho}\right] + \sum_j \kappa_j \int d^3\mathbf{r}\mathscr{L}_j\left[\hat{\rho}\right]$$

- Here the Liouville terms describe coupling to the reservoirs:

$$\mathscr{L}_j\left[\hat{\rho}\right] = 2\hat{O}_j\hat{\rho}\,\hat{O}_j^\dagger - \hat{O}_j^\dagger\hat{O}_j\hat{\rho} - \hat{\rho}\,\hat{O}_j^\dagger\hat{O}_j$$

- For n-particle collisions: $\hat{O}_i = \left[\widehat{\Psi}_i(\mathbf{r})\right]^n$

Truncated Wigner equations for the BEC case

Result of operator mappings + truncation - for the GPE:

$$\frac{d\alpha_i}{dt} = -i\sum_j \left[\omega_{ij}\alpha_j + \chi_{ij}|\alpha_j|^2\alpha_i\right] - \gamma_i\alpha_i + \sqrt{\gamma_i}\zeta_i(t)$$

$\zeta_i(t)$ is a complex, stochastic delta-correlated Gaussian noise:

$$\left\langle \zeta_i(t)\zeta_j^*(t')\right\rangle = \delta_{ij}\delta\left(t - t'\right).$$

Initial fluctuations: $\langle \Delta\alpha_i \Delta\alpha_i^* \rangle = \frac{1}{2}\delta_{ij}$

First-principle simulations

What do we do with modes having low occupation numbers?

- Truncated Wigner only works if all modes are heavily occupied
- How about modeling other cases with low occupations:
  - the formation of a BEC must start with low occupation!
  - collisions that generate atoms in initially empty modes
  - coupling to thermal modes having low occupation?
- We need a technique without the large N approximation

+P PHASE-SPACE METHODS

The positive P-representation is an expansion in coherent state projectors

$$\widehat{\rho} = \int P(\boldsymbol{\alpha},\boldsymbol{\beta})\widehat{\Lambda}(\boldsymbol{\alpha},\boldsymbol{\beta})d^{2M}\boldsymbol{\alpha}\, d^{2M}\boldsymbol{\beta}$$

$$\widehat{\Lambda}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}^*|}{\langle\boldsymbol{\beta}^*||\boldsymbol{\alpha}\rangle}$$

Enlarged phase-space allows positive probabilities!

- Maps quantum states into 4M real coordinates: $\boldsymbol{\alpha},\boldsymbol{\beta} = \mathbf{p} + i\mathbf{x}, \mathbf{p}' + i\mathbf{x}'$
- Double the size of a classical phase-space
- Exact mappings even for low occupations

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+P Existence Theorem

For ANY density matrix, a positive P-function always exists

$$P(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{(2\pi)^{2M}} e^{-\left|\boldsymbol{\alpha}-\boldsymbol{\beta}^*\right|^2/4} \left\langle \frac{\boldsymbol{\alpha}+\boldsymbol{\beta}^*}{2} \right| \widehat{\rho} \left| \frac{\boldsymbol{\alpha}+\boldsymbol{\beta}^*}{2} \right\rangle$$

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- Problem: Non-uniqueness allows sampling error to grows with time (chaotic)

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Operator identities

Differentiating the projection operator gives the following identities

$$
\begin{aligned}
\widehat{a}_n^\dagger \widehat{\rho} &\rightarrow \left[\beta_n - \frac{\partial}{\partial \alpha_n}\right] P \\
\widehat{a}_n \widehat{\rho} &\rightarrow \alpha_n P \\
\widehat{\rho}\,\widehat{a}_n &\rightarrow \left[\alpha_n - \frac{\partial}{\partial \beta_n}\right] P \\
\widehat{\rho}\,\widehat{a}_n^\dagger &\rightarrow \beta_n P
\end{aligned}
$$

Since the projector is an analytic function of both α_n and β_n, we can obtain alternate identities by replacing $\partial/\partial\alpha$ by either $\partial/\partial\alpha_x$ or $\partial/i\partial\alpha_y$. This equivalence allows a positive-definite diffusion to be obtained, with stochastic evolution.

Measurements

How do we calculate an operator expectation value

- There is a correspondence between the moments of the distribution, and the normally ordered operator products.
- These come from the fact that coherent states are eigenstates of the annihilation operator
- Using $\mathrm{Tr}\left[\widehat{\Lambda}(\boldsymbol{\alpha},\boldsymbol{\beta})\right] = 1$:

$$\langle \widehat{a}_m^\dagger \cdots \widehat{a}_n \rangle = \int\int P(\boldsymbol{\alpha},\boldsymbol{\beta})[\beta_m \cdots \alpha_n] d^{2M}\boldsymbol{\alpha}\, d^{2M}\boldsymbol{\beta}\,.$$

General case

Suppose we have a more general Hamiltonian, like the BEC case. Then we define

$$\overrightarrow{\alpha} = (\boldsymbol{\alpha}, \boldsymbol{\beta})$$

and find using operator mappings that - provided the distribution is sufficiently bounded at infinity:

$$\frac{\partial}{\partial t} P(t, \overrightarrow{\alpha}) = \left[\partial_i A_i(\overrightarrow{\alpha}) + \frac{1}{2} \partial_i \partial_j D_{ij}(t, \overrightarrow{\alpha}) \right] P(t, \overrightarrow{\alpha}) \, .$$

Comparison of positive-P and Wigner

- There are no other terms in +P - higher order derivatives all vanish
- Nonlinear couplings cause noise, linear damping does not

+P equations for the BEC case

Exact result of operator mappings - assume χ_{ij} is diagonal for simplicity

$$\frac{d\alpha_i}{dt} = -i\sum_j \left[\omega_{ij}\alpha_j + \chi_i\beta_i\alpha_i^2\right] - \gamma_i\alpha_i + \sqrt{-i\chi_i}\,\alpha_i\zeta_i(t)$$

$$\frac{d\beta_i}{dt} = i\sum_j \left[\omega_{ij}\beta_j + \chi_i\beta_i^2\alpha_i\right] - \gamma_i\beta_i + \sqrt{i\chi_i}\,\beta_i\zeta_{M+i}(t)$$

$\zeta_i(t)$ is a complex, stochastic delta-correlated Gaussian noise:

$$\left\langle \zeta_i(t)\zeta_j(t')\right\rangle = \delta_{ij}\delta\left(t - t'\right).$$

Initial fluctuations in a coherent state: $\langle \Delta\alpha_i \Delta\alpha_i^* \rangle = 0$

+P equations in an optical lattice

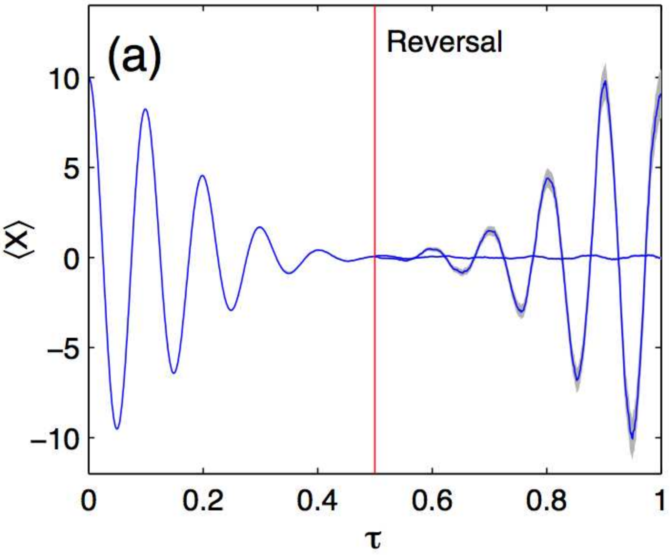
Single mode case of an anharmonic oscillator

$$\frac{d\alpha}{dt} = -i\chi\alpha^2\beta + \sqrt{-i\chi}\,\alpha\zeta_1(t)$$
$$\frac{d\beta}{dt} = i\chi\beta^2\alpha + \sqrt{i\chi}\,\beta\zeta_2(t)$$

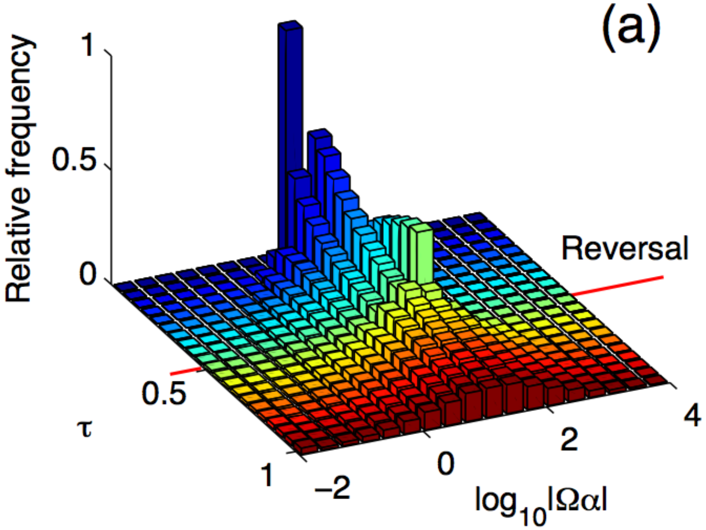
$\zeta_i(t)$ is a complex, stochastic delta-correlated Gaussian noise:
$\langle\zeta_i(t)\zeta_j(t')\rangle = \delta_{ij}\delta\left(t-t'\right)$.

- What happens if we change the sign of χ?
- This is the same as changing the sign of H , or reversing the time-direction.
- Quantum mechanics is reversible - how can a stochastic process be reversible?

Time-reversal test: up to 10^{23} interacting bosons



Phase-space distribution is not unique!



+P equations for evaporative cooling

Two or three-dimensional simulations

- Consider 10000 atoms in 32000 trap modes
- 10^{300} states in Hilbert space
- Evaporative cooling: strong damping at edges of trap
- Full quantum dynamics can be simulated
- This is a nonequilibrium problem, no thermal reservoirs present
- **What final quantum state is produced?**

+P simulation results

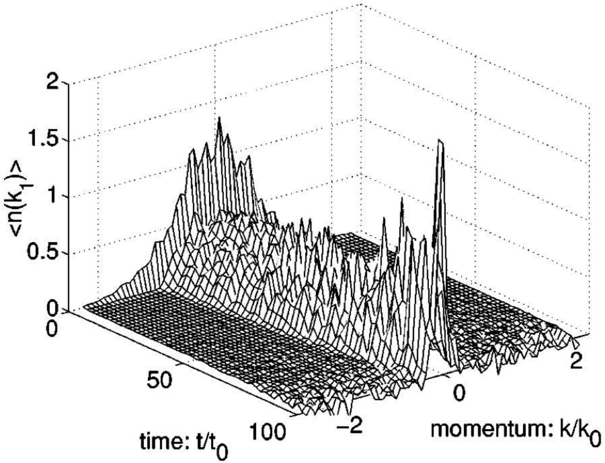
Two or three-dimensional simulations

- Consider density distributions in momentum space
- Confinement defined as:

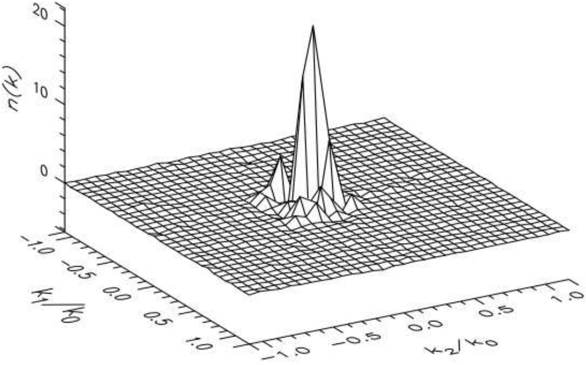
$$Q = \frac{\int d^3\mathbf{k} \left\langle \alpha^2(\mathbf{k})\beta^2(\mathbf{k}) \right\rangle}{x_0^3 \left[\int d^3\mathbf{k} \left\langle \alpha(\mathbf{k})\beta(\mathbf{k}) \right\rangle\right]^2}$$

- Sharp rise in confinement: BEC formation
- Evidence of finite COM motion
- Evidence of finite angular momentum

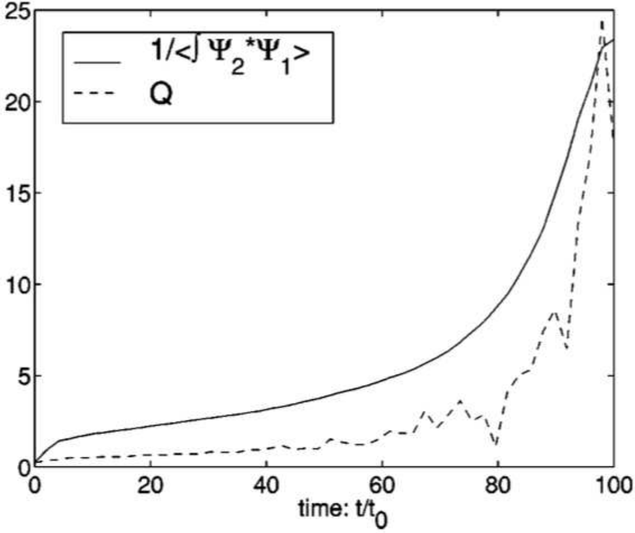
BEC formation in 2D



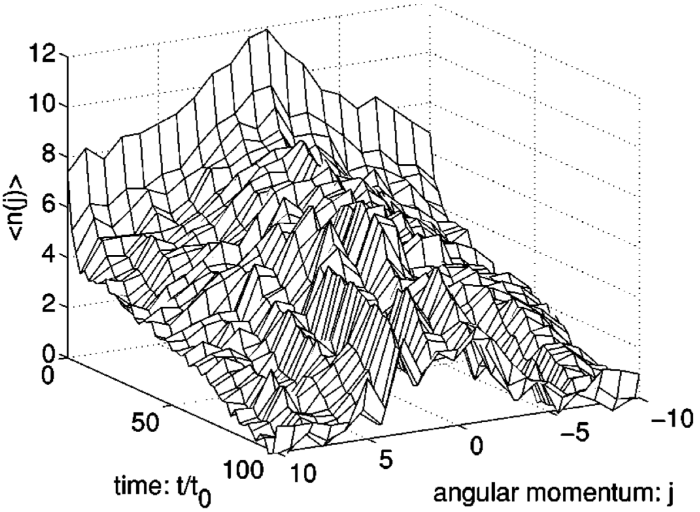
BEC formation in 3D



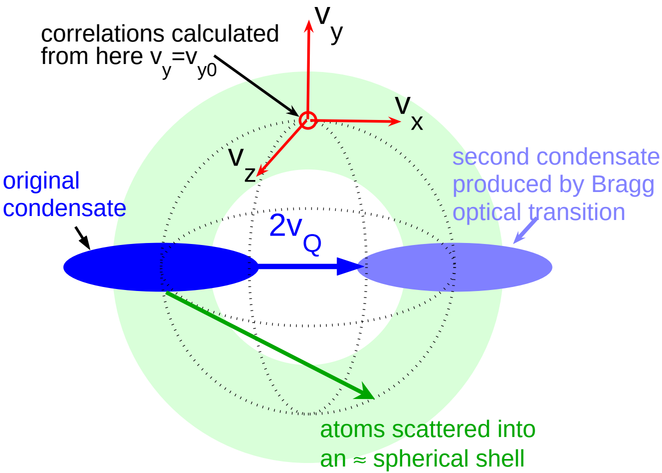
Confinement in 3D



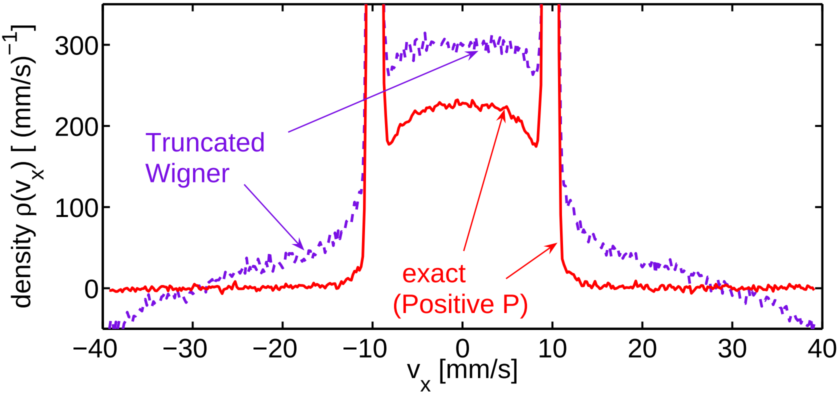
Vortex formation in 2D



BEC collision: 10^5 bosons, 10^6 spatial modes



Positive-P vs Truncated Wigner



3D Truncated Wigner: diverges, +P: converges

+P advantages and drawbacks

- Advantage: Can treat exponentially large systems
- First-principles approach WITHOUT factorization assumption
- No truncation
- No UV divergence at large k-value
- Drawback: Sampling error grows in time
- **Can't simulate unitary evolution for long times!**

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