Phase-space methods for quantum simulations

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The problem: complexity

How can we calculate quantum dynamics?

**BEC:** \(10^{100000}\) states, \(10^6\) qubits in Hilbert space

- Real time path integrals don’t converge
- Mean field methods don’t give quantum statistics
- Direct computation needs don’t fit into memory!
Phase-space representations

✓ Quantum dynamics → stochastic motion + sampling

✗ Classical phase-space: **Wigner**, **P-**, **Q**, $d$ dimensions

✓ Quantum phase-space: **Positive-P**, $2d$ dimensions

✓ Stochastic gauge: adds a weight to the trajectory
Phase-Space Representations

Expand the density matrix $\hat{\rho}$, using operators $\hat{\Lambda}(\vec{\lambda})$:

$$\hat{\rho} = \int P(\vec{\lambda})\hat{\Lambda}(\vec{\lambda})d\vec{\lambda}$$

Quantum dynamics $\rightarrow$ Trajectories in $\vec{\lambda}$.

Different basis choice $\hat{\Lambda}(\vec{\lambda}) \rightarrow$ different representation
General $M$-mode Gaussian operator

Normally-ordered exponential of a general quadratic form in the $2M$-vector mode operator $\delta \hat{a} = (\hat{a}, \hat{a}^\dagger) - \alpha$, where $\alpha$ is a $2M$-vector c-number and $\hat{a}$ is the vector of annihilation operators. For algebraic reasons, it is useful to employ normal ordering, and to introduce a compact notation using a generalized covariance $\Sigma$:

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

In this case, the phase-space is described by the complex variables $\lambda = (\Omega, \alpha, \Sigma) = (\Omega, \alpha)$. 
What is the covariance?

\[ \sigma = \begin{bmatrix} \mathbf{I} + \mathbf{n} & \mathbf{m} \\ \mathbf{m}^+ & \mathbf{I} + \mathbf{n}^T \end{bmatrix}. \]

The representation phase space is \( \vec{\lambda} = (\Omega, \alpha, \alpha^+, \mathbf{n}, \mathbf{m}, \mathbf{m}^+) \)

- \( \Omega \) = weight factor
- \( \alpha, \alpha^+ \) = amplitude
- \( \mathbf{n} \) = number correlation (complex \( M \times M \) matrix).
- \( \mathbf{m}, \mathbf{m}^+ \) = squeezing (symmetric complex \( M \times M \) matrices)
What are the moments physically?

\[
\begin{align*}
\langle \hat{a}_i \rangle &= \langle \Omega \alpha_i \rangle_p \\
\langle \hat{a}_i^\dagger \rangle &= \langle \Omega \alpha_i^\dagger \rangle_p \\
\langle \hat{a}_i \hat{a}_j \rangle &= \langle \Omega (\alpha_i \alpha_j + m_{ij}) \rangle_p \\
\langle :\hat{a}_i \hat{a}_j^\dagger : \rangle &= \langle \Omega (\alpha_i \alpha_j^\dagger + n_{ij}) \rangle_p \\
\langle \hat{a}_i^\dagger \hat{a}_j^\dagger \rangle &= \langle \Omega (\alpha_i^\dagger \alpha_j^\dagger + m_{ij}^\dagger) \rangle_p .
\end{align*}
\]
Standard Phase-space Representations

What about the text-book phase-space representations?

<table>
<thead>
<tr>
<th>Property: Repn.</th>
<th>Variance ((n))</th>
<th>Operator Order</th>
<th>Phase-space</th>
</tr>
</thead>
<tbody>
<tr>
<td>(P)</td>
<td>0</td>
<td>Normal</td>
<td>Classical</td>
</tr>
<tr>
<td>(W)</td>
<td>1/2</td>
<td>Symmetric</td>
<td>Classical</td>
</tr>
<tr>
<td>(Q)</td>
<td>1</td>
<td>Antinormal</td>
<td>Classical</td>
</tr>
<tr>
<td>(+P)</td>
<td>0</td>
<td>Normal</td>
<td>Classical (\times2)</td>
</tr>
<tr>
<td>(G)</td>
<td>(n)</td>
<td>Any</td>
<td>((\text{Classical})^2)</td>
</tr>
</tbody>
</table>
There are three main types of problems studied:

- Master equations - damping + coherent evolution
- Canonical ensembles - ‘imaginary time’ thermal equilibrium
- Quantum dynamics - purely coherent nonlinear evolution
1. **PROBLEM:** $\partial \hat{\rho} / \partial t = \hat{L}[\hat{\rho}]$

2. Define: $p$-dimensional complex space: $\overrightarrow{\lambda} = (\Omega, \alpha)$

3. **Basis** $\hat{\Lambda}(\overrightarrow{\lambda})$: $\hat{\rho} = \int P(\overrightarrow{\lambda}) \hat{\Lambda}(\overrightarrow{\lambda}) d^{2p} \overrightarrow{\lambda}$

4. Identities: $\partial \hat{\rho} / \partial t = \int P(\overrightarrow{\lambda}) \hat{L}[\hat{\Lambda}(\overrightarrow{\lambda})] d^{2p} \overrightarrow{\lambda}$

5. **Diffusion and drift gauge:** $g^d(\alpha), g(\alpha)$

6. **STOCHASTICS:**
   - $d\Omega / \partial t = \Omega [U + g \cdot \zeta]$
   - $d\alpha / \partial t = A + B(\zeta - g)$
CENTRAL RESULT

Stochastic equations: trajectory $\alpha$, quantum amplitude $\Omega$:

Gauge  \[ \frac{d\Omega}{dt} = \Omega [U dt + g(\alpha) \cdot \zeta(t)] \]

Trajectory  \[ \frac{d\alpha}{dt} = A + B[\zeta(t) - g(\alpha)] \]

- Noise correlations:  \[ \langle \zeta_i(t)\zeta_j(t') \rangle = \delta_{ij}\delta(t - t') \]

- Gauges chosen freely to optimize simulations

- Provided no boundary terms, all gauges EQUIVALENT

- Works for either bosons or fermions

- Sign changes for fermions and NO amplitude terms
COMPUTATIONAL STRATEGIES

- BASIS SET
- GAUGE
- ALGORITHM
# League Table of Representations

How do the known phase-space representations compare?

<table>
<thead>
<tr>
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<tr>
<td>W</td>
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</table>
I: CANONICAL BOSE-HUBBARD MODEL

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

\[ \hat{H}(a, a^\dagger) = \hbar \left[ \sum \sum \omega_{ij} a_i^\dagger a_j + \sum : n_j^2 : \right]. \]

- \( \omega_{ij} \) - nonlocal coupling, includes chemical potential.
- Boson number: \( \hat{n}_i = a_i^\dagger a_i \).
- Grand canonical ensemble: \( \hat{\rho}_u = e^{-(\hat{H} - \mu \hat{N})/k_BT} = e^{-\hat{K}\tau} \).
Stochastic gauge equations

Choose \( n = 0 \) then → Imaginary time Gross- Pitaevskii equations with weighting and quantum noise:

\[
\frac{d\alpha_i}{d\tau} = - \left[ \alpha_i^\dagger \alpha_i + i \omega_i \right] \alpha_i - \sum_{j=1}^{M} \omega_{ij} \alpha_j / 2 + i \alpha_i \xi_i(\tau)
\]

\[
\frac{d\Omega}{d\tau} = \left[ -K(\tau)d\tau + \sum_{i=1}^{M} g_i \xi_i(\tau) \right] \Omega
\]

STABILISING GAUGE: \( g_j = i(Re(\alpha_i^\dagger \alpha_i) - |\alpha_i^\dagger \alpha_i|) \),
Single-well, interacting case

Antibunching: single Bose mode,
NOTE: $\tau = \text{Inverse temperature}$
Simulations vs exact energy and density

✓ Complete agreement with exact solutions
  - at all temperatures calculated!
Spatial correlations, $g^{(2)}(x)$ can be calculated from gauge simulations:

1 Dimensional interacting Bose Gas
Interaction strength $c = 1$

$z(T) = e^{\mu T} = z_0 + (z_\pi - z_0)(1 - \cos(1/T))/2$
$z_0 = \exp(-8)$
$z_\pi = \exp(-1)$

25 000 trajectories
$\Delta t = 0.005$
Lattice Size = 750
System Length = 180
II: REAL-TIME BOSE-HUBBARD MODEL

- $n = 0$ (positive-$P$) $\rightarrow$ Real time Gross- Pitaevskii equations with quantum noise:

$$\frac{d\alpha_i}{dt} = -i \left[ n_i + \sum_{j=1}^{2M} \omega_{ij} \alpha_j + \sqrt{i} \xi_i(\tau) \right] \alpha_i$$

- $n = 1/2$ (Wigner) $\rightarrow$ Approximate Gross- Pitaevskii equations with $\langle \alpha_i^0 \alpha_i^0 \rangle = 1/2$

$$\frac{d\alpha_i}{dt} = -i \left[ n_i + \sum_{j=1}^{2M} \omega_{ij} \alpha_j \right] \alpha_i$$
BEC evaporative cooling (1998): $10^5$ qubits
III: NONCLASSICAL QUANTUM DYNAMICS:

Coherent molecular down-conversion

• Coherent process of molecular dissociation

• Overall effective Hamiltonian term in one dimension of

\[
\hat{H} = \hat{H}_0 + \frac{i\hbar \chi(t)}{2} \int dx \left[ e^{i\omega t} \Psi_2^\dagger \Psi_1^2 - e^{-i\omega t} \Psi_2 \Psi_1^2 \right],
\]

• \(\chi(t)\) is the bare atom-molecule coupling; \(\omega\) is a detuning
Stochastic Equations

\[
\frac{\partial \psi_1}{\partial \tau} = i \frac{\partial^2 \psi_1}{\partial \xi^2} - (\gamma + i \delta) \psi_1 + \kappa \psi_2 \psi_1^+ + \sqrt{\kappa \psi_2 \eta_1},
\]

\[
\frac{\partial \psi_1^+}{\partial \tau} = -i \frac{\partial^2 \psi_1^+}{\partial \xi^2} - (\gamma - i \delta) \psi_1^+ + \kappa \psi_2^+ \psi + \sqrt{\kappa \psi_2 \eta_1^+},
\]

\[
\frac{\partial \psi_2}{\partial \tau} = \frac{i}{2} \frac{\partial^2 \psi_2}{\partial \xi^2} - i v(\xi, \tau) \psi_2 - \frac{\kappa}{2} \psi_1^2 + \sqrt{-i \nu \psi_2 \eta_2},
\]

\[
\frac{\partial \psi_2^+}{\partial \tau} = -\frac{i}{2} \frac{\partial^2 \psi_2^+}{\partial \xi^2} + i v(\xi, \tau) \psi_2^+ - \frac{\kappa}{2} \psi_1^{+2} + \sqrt{i \nu \psi_2^+ \eta_2^+}.
\]
Twin atom correlations
We have a new Australian Research Council Centre of Excellence in Quantum Atom Optics - with open theoretical and experimental positions for graduate students and postdocs - at:

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✅ MELBOURNE

SEE: WWW.ACQAO.ORG

(Free software: WWW.XMDS.ORG)