Simulating photons, atoms and molecules with quantum phase-space methods

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ACQAO Theory @ UQ

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Simplicity of Photons and Ultracold Gases

✔ underlying interactions are well understood

✔ easily characterised by a few parameters

✔ interactions can be tuned

$\longrightarrow$ use simple theoretical models to high accuracy

$\longrightarrow$ develop and test new methods of calculation

Theoretical Methods

- deterministic methods:
  - ➜ exact diagonalisation ✗ intractable for $\gtrsim 5$ particles
  - ➜ factorization ✗ not applicable for strong correlations
  - ➜ perturbation theory ✗ diverges at strong couplings
  - ➜ density functional theory ✗ introduces approximations
- probablistic methods:
  - ➜ quantum Monte Carlo (QMC)
  - ➜ stochastic wavefunction
  - ➜ phase-space methods

Overview

- introduction to phase-space representations
- density operator description of quantum evolution (3 classes)
  - ➜ static, unitary and open
- Gaussian operator bases (3 types)
  - ➜ coherent, thermal and squeezed
- applications (3 examples)
  - ➜ pulse propagation in optical fibres *(photons)*
  - ➜ Hubbard model *(atoms)*
  - ➜ simple atomic-molecular dynamics *(molecules)*

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Phase-space distributions

- A classical state can be represented by a joint probability distribution in phase space $P(\mathbf{x},\mathbf{p})$

- 1932: Wigner constructed an analogous quantity for a quantum state:

$$W(x,p) = \frac{2}{\pi}\int dy \psi^*(x-y)\,\psi(x+y)\exp(-2iyp/\hbar)$$

✔ Wigner function gives correct marginals: $\int dx W(x,p) = 2\hbar P(p)$, $\int dy W(x,p) = 2\hbar P(x)$

✘ but it is not always positive $\longrightarrow$ not a true joint probability

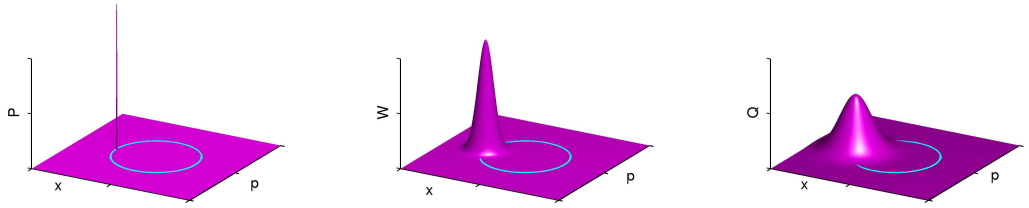
- a positive Wigner function would mean a hidden variable interpretation of QM is valid

Probability distributions

- many ways to define phase-space distributions:
  - ➜ eg Wigner, Husimi Q and Glauber-Sudarshan P
    - ☛ all defined in terms of coherent states
    - ☛ correspond to different choices of orderings

- to be a probabilistic representation, the phase-space functions must:

	P	W	Q
exist and be nonsingular	✘	✔	✔
always be positive	✘	✘	✔
evolve via drift and diffusion	✘	✘	✘



Reversibility

- classical random process is irreversible
  - ➜ outward (positive) diffusion
- quantum mechanics is reversible
  - ➜ phase-space functions generally don’t have positive diffusion

A solution!

- dimension doubling
  - ➜ diffusion into ’imaginary’ dimensions ✔
  - ➜ observables evolve reversibly ✔
  - ➜ also fixes up existence and positivity ✔

Phase-space representation

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

- $P(\vec{\lambda})$ is a probability distribution
- $\hat{\Lambda}(\vec{\lambda})$ is a suitable operator basis
- $\vec{\lambda}$ is a generalised phase-space coordinate
- $d\vec{\lambda}$ is an integration measure
- equivalent to

$$\hat{\rho} = E\left[\hat{\Lambda}(\vec{\lambda})\right]$$

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Many-body quantum state

- Most general description is given by a density operator: $\hat{\rho}$
- Encapsulates all correlations in a quantum state:

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}\left\{ \hat{O}\hat{\rho} \right\}$$

- A probabilistic expansion in the eigenbasis:

$$\hat{\rho} = \sum_k P_k \left| \Psi_k \right\rangle \left\langle \Psi_k \right|$$

Density operators for quantum evolution

1. Unitary dynamics: $\widehat{\rho}(t) = e^{-i\widehat{H}t/\hbar}\widehat{\rho}(0)e^{i\widehat{H}t/\hbar}$
   - $\frac{\partial}{\partial t}\widehat{\rho} = -\frac{i}{\hbar}\left[\widehat{H},\widehat{\rho}\right]$
2. Equilibrium state: $\widehat{\rho}_{\mathrm{un}}(T) = e^{-\left(\widehat{H}-\mu\widehat{N}\right)/k_BT}$
   - $\frac{\partial}{\partial \tau} = \frac{1}{2}\left[\widehat{H}-\mu\widehat{N},\widehat{\rho}\right]_+ ; \tau = 1/k_BT$
3. Open dynamics: $\widehat{\rho}_{\mathrm{Sys}} = \mathrm{Tr}_{\mathrm{Res}}\{\widehat{\rho}\}$
   - $\frac{\partial}{\partial t}\widehat{\rho} = -\frac{i}{\hbar}\left[\widehat{H},\widehat{\rho}\right] + \gamma\left(2\widehat{R}\widehat{\rho}\widehat{R}^\dagger - \widehat{R}^\dagger\widehat{R}\widehat{\rho} - \widehat{\rho}\widehat{R}^\dagger\widehat{R}\right)$

- each type is equivalent to a Liouville equation for $\widehat{\rho}$:

$$\frac{d}{d\tau}\widehat{\rho} \;=\; \widehat{L}\left[\widehat{\rho}\right]$$

Phase-space Recipe

1. **Formulate**: $\partial\widehat{\rho}/\partial\tau = \widehat{L}[\widehat{\rho}]$
2. **Expand**: $\int \partial P/\partial\tau \widehat{\Lambda} d\overrightarrow{\lambda} = \int P\widehat{L}\left[\widehat{\Lambda}\right] d\overrightarrow{\lambda}$
3. **Transform**: $\widehat{L}\left[\widehat{\Lambda}\right] = \mathcal{L}\widehat{\Lambda}$
4. **Integrate** by parts: $\int P\,\mathcal{L}\widehat{\Lambda} d\overrightarrow{\lambda} \Longrightarrow \int \widehat{\Lambda}\,\mathcal{L}'P\,d\overrightarrow{\lambda}$
5. **Obtain** Fokker-Planck equation: $\partial P/\partial\tau = \mathcal{L}'P$
6. **Sample** with stochastic equations for $\overrightarrow{\lambda}$

Stochastic Gauges

- Mapping from Hilbert space to phase space not unique

  ➜ many “gauge” choices

- Can alter noise terms B_{ij}, introduce arbitrary drift functions $g_j(\vec{\lambda})$

Weight $d\Omega/d\tau = \Omega\left[U + g_j\,\zeta_j\right]$

Trajectory $d\lambda_i/\partial\tau = A_i + B_{ij}[\zeta_j - g_j]$

Interacting many-body physics

$$\hat{\rho} \Longrightarrow \overrightarrow{\lambda}$$

- ✔ many-body problems map to nonlinear stochastic equations
- ✔ calculations can be from first-principles
- ✔ precision limited only by sampling error
- ✔ choose basis to suit the problem

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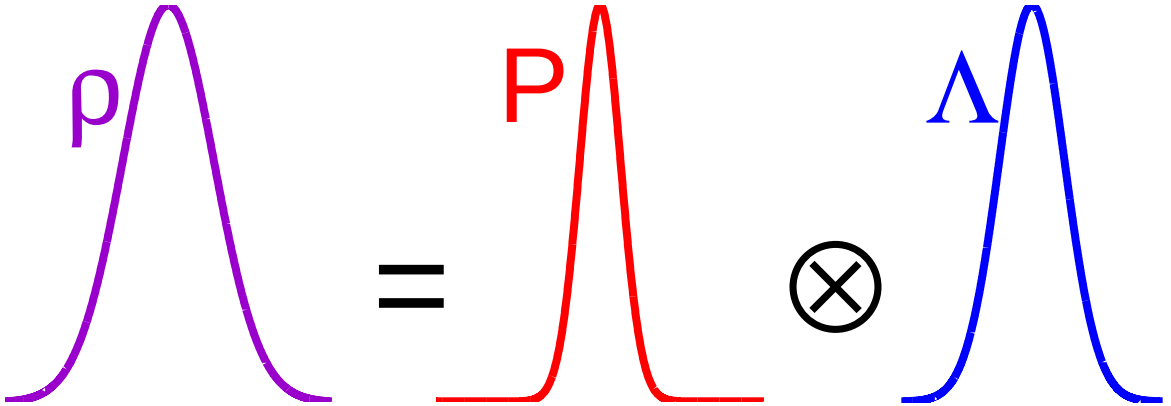
Operator Bases

- need basis simple enough to fit into a computer, complex enough to contain the relevant physics:

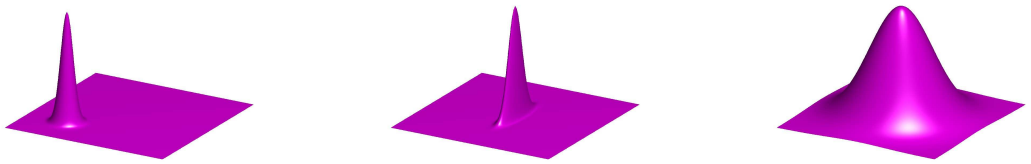


$$\sigma_\rho \sim \sigma_P + \sigma_\Lambda$$

General Gaussian operators

a generalisation of the density operators that describe Gaussian states

- Gaussian states can be:
  - ➜ coherent (for bosons), squeezed, or thermal



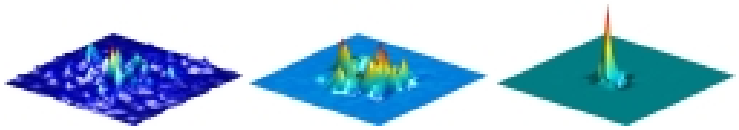
  - ➜ or any combination of these
- characterised by first-order moments: $\overline{x}$, $\overline{p}$, $\overline{x^2}$, $\overline{p^2}$, $\overline{xp}$
  - ➜ all higher-order moments factorise

Gaussian Basis I: Coherent-state projectors

$$\widehat{\Lambda} = \frac{|\alpha\rangle\langle\beta|}{\langle\beta||\alpha\rangle}$$

- defines the $+P$ distribution, with a doubled phase space $\overrightarrow{\lambda} = (\Omega, \alpha, \beta)$
- moments: $\left\langle O\left(\widehat{\mathbf{a}}^{\dagger}, \widehat{\mathbf{a}}\right)\right\rangle = E\left[O\left(\beta^{*}, \alpha\right)\right]$
- successful for many applications in quantum optics
- successful simulations of short-time quantum dynamics of BEC

Evaporative Cooling of a BEC



❄ first-principles 3D calculation

➜ start with Bose gas above T_c; finish with narrow BEC peak

➜ 20000 atoms, 32000 modes

➜ Hilbert space is astronomically large

✘ Problems!

✘ method pushed to the limit

✘ breaks down for longer times, stronger interactions

Gaussian Basis II: Thermal operators

$$\widehat{\Lambda} = |\mathbf{I} \pm \mathbf{n}|^{\mp 1} : \exp\left[\widehat{\mathbf{a}}\left(\mathbf{I} \mp \mathbf{I} - [\mathbf{I} \pm \mathbf{n}]^{-1}\right)\widehat{\mathbf{a}}^{\dagger}\right] :$$

- now have a phase-space of variances: $\overrightarrow{\lambda} = (\Omega, \mathbf{n})$
- defined for bosons (upper sign) and *fermions* (lower sign)
- moments: $\left\langle \widehat{a}_i^{\dagger}\widehat{a}_j \right\rangle = E\left[n_{ij}\right]$, $\left\langle \widehat{a}_i^{\dagger}\widehat{a}_j^{\dagger}\widehat{a}_j\widehat{a}_i \right\rangle = E\left[n_{ii}n_{jj} - n_{ij}n_{ji}\right]$
- suitable for cold atoms

Gaussian Basis III: General form (including squeezing)

$$\widehat{\Lambda}(\overrightarrow{\lambda}) = \Omega \sqrt{\left|\underline{\underline{\sigma}}\right|^{\mp 1}} : \exp\left[\delta\underline{\widehat{a}}^{\dagger}\left(\underline{\underline{I}} \mp \underline{\underline{I}} - \underline{\underline{\sigma}}^{-1}\right)\delta\underline{\widehat{a}}/2\right] :$$

relative displacement: $\delta\underline{\widehat{a}} = \underline{\widehat{a}} - \underline{\alpha}$

annihilation and creation operators: $\underline{\widehat{a}} = \left(\widehat{a}_1, \ldots, \widehat{a}_M, \widehat{a}_1^{\dagger}, \ldots, \widehat{a}_M^{\dagger}\right)$

coherent offset: $\underline{\alpha} = \left(\alpha_1, \ldots, \alpha_M, \alpha_1^{+}, \ldots, \alpha_M^{+}\right)$, ($\underline{\alpha} = 0$ for fermions)

covariance: $\underline{\underline{\sigma}} = \begin{bmatrix} \mathbf{n}^T \pm \mathbf{I} & \mathbf{m} \\ \mathbf{m}^{+} & \mathbf{I} \pm \mathbf{n} \end{bmatrix}, \underline{\underline{I}} = \begin{bmatrix} \pm\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}.$

upper signs: bosons; **lower signs:** fermions

Extended phase space

$$\overrightarrow{\lambda} \quad = \quad (\Omega, \alpha, \alpha^+, \mathbf{n}, \mathbf{m}, \mathbf{m}^+)$$

$\Longrightarrow$ Hilbert-space dimension: 2^M for fermions, N^M for bosons

$\Longrightarrow$ phase-space dimension: $2(1-M+2M^2)$ for fermions, $2(1+3M+2M^2)$ for bosons

❄ Moments:

$$\langle \widehat{a}_i \rangle = \langle \alpha_i \rangle_P$$
$$\left\langle \widehat{a}_i^\dagger \widehat{a}_j \right\rangle = \langle \alpha_i^+ \alpha_j \rangle_P + \langle n_{ij} \rangle_P$$
$$\langle \widehat{a}_i \widehat{a}_j \rangle = \langle \alpha_i \alpha_j \rangle_P + \langle m_{ij} \rangle_P$$

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Application I: photons in a fibre

$$\widehat{H} = \widehat{H}_F + \widehat{H}_L + \widehat{H}_G + \widehat{H}_R$$

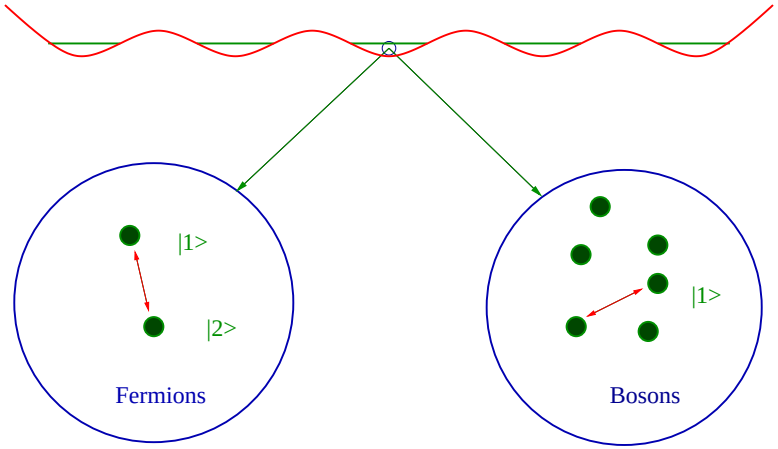
- $\widehat{H}_F$:fibre-optic Hamiltonian, including $\chi^{(3)}$nonlinearity
- $\widehat{H}_L$, $\widehat{H}_G$: coupling to absorbing reserviors and fibre amplifier reserviors
- $\widehat{H}_R$: nonlinear coupling to non-Markovian phonon reserviors
- have 10^2 modes and 10^9 particles

Phase-Space Equations

- use coherent-state basis $\longrightarrow$ get a stochastic, Raman modified NLS equations:

$$\begin{aligned}
\frac{\partial}{\partial x}\phi(t,x) &= -\int_{-\infty}^{\infty} dt' g(t-t')\phi(t',x) + \Gamma(t,x) \pm \frac{i}{2}\frac{\partial^2}{\partial t^2}\phi \\
&\quad + \left[i\int_{-\infty}^{\infty} dt' h(t-t')\phi^{+}(t',x)\phi(t',x) + \Gamma^{R}(t,x) \right] \phi(t,x) \\
\frac{\partial}{\partial x}\phi^{+}(t,x) &= -\int_{-\infty}^{\infty} dt' g^{*}(t-t')\phi^{+}(t',x) + \Gamma^{+}(t,x) \mp \frac{i}{2}\frac{\partial^2}{\partial t^2}\phi \\
&\quad + \left[i\int_{-\infty}^{\infty} dt' h^{*}(t-t')\phi(t',x)\phi^{+}(t',x) + \Gamma^{+R}(t,x) \right] \phi^{+}(t,x)
\end{aligned}$$

Application II: atoms in a lattice



$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{a}^{\dagger}_{i,\sigma} \hat{a}_{j,\sigma} + U \sum_{j} \hat{a}^{\dagger}_{j,\uparrow} \hat{a}^{\dagger}_{j,\downarrow} \hat{a}_{j,\downarrow} \hat{a}_{j,\uparrow}$$

- simplest model of an interacting Fermi gas on a lattice

  ➜ weak-coupling limit $\longrightarrow$ BCS transitions

  ➜ solid-state models; relevance to High-T_c superconductors

Solving the Hubbard Model

- ❄ only the 1D model is exactly solvable (Lieb & Wu, 1968)
- ❄ even then, not all correlations can be calculated
- ❄ higher dimensions - can use Quantum Monte Carlo methods.
- ✘ except for a few special symmetrical cases, QMC suffers from sign problems with the Hubbard model
  - ❄ e.g. sign problems for repulsive interaction away from half filling
- ✘ sign problem increases with dimension, lattice size, interaction strength

Fermionic sign problem

- Quantum Monte Carlo (QMC) samples many-body wavefunction $\phi(r)$ (wavefunction treated as a probability)

- but Fermion states are antisymmetric

  ➜ wavefunction nonpositive

- must introduce (possibly negative) weighting factors

  ➜ bad sampling errors (unless approximations used)

$$\langle A \rangle \sim \frac{\langle sA \rangle}{\langle s \rangle}$$

Applying the Gaussian representation

❄ Use thermal basis, and apply mappings

$$\hat{\mathbf{n}}_\sigma\hat{\rho} \rightarrow \left\{2\mathbf{n}_\sigma - (\mathbf{I}-\mathbf{n}_\sigma)\frac{\partial}{\partial \mathbf{n}_\sigma}\mathbf{n}_\sigma\right\} P(\Omega,\mathbf{n}_\uparrow,\mathbf{n}_\downarrow)$$

$$\hat{\rho}\hat{\mathbf{n}}_\sigma \rightarrow \left\{2\mathbf{n}_\sigma - \mathbf{I} - \mathbf{n}_\sigma\frac{\partial}{\partial \mathbf{n}_\sigma}(\mathbf{I}-\mathbf{n}_\sigma)\right\} P(\Omega,\mathbf{n}_\uparrow,\mathbf{n}_\downarrow)$$

$$\hat{\rho} \rightarrow -\frac{\partial}{\partial\Omega}\Omega(\Omega,\mathbf{n}_\uparrow,\mathbf{n}_\downarrow)$$

$\Longrightarrow$ Fokker-Planck equation for P, with drift and diffusion

$\Longrightarrow$ sample with stochastic equations for Ω and $\mathbf{n}_\sigma$

Positive-Definite Diffusion

❄ Modify interaction term with a ‘Fermi gauge’:

$$U\sum_j :\hat{n}_{jj,\downarrow}\hat{n}_{jj,\uparrow}: \;=\; -\frac{1}{2}|U|\sum_j :\left(\hat{n}_{jj,\downarrow}-\frac{U}{|U|}\hat{n}_{jj,\uparrow}\right)^2:$$

$\Longrightarrow$ diffusion matrix has a real ’square root’ matrix

$\Longrightarrow$ realise the diffusion with a real noise process

$\Longrightarrow$ problem maps to a real (and much more stable) subspace

Stratonovich Equations

- Stratonovich stochastic equations, in matrix form:

$$\frac{d\Omega}{d\tau} = -\Omega\left\{-t\sum_{\langle i,j\rangle,\sigma} n_{ij,\sigma} + U\sum_{j} n_{jj,\downarrow}n_{jj,\uparrow} - \mu\sum_{j,\sigma} n_{jj,\sigma}\right\}$$

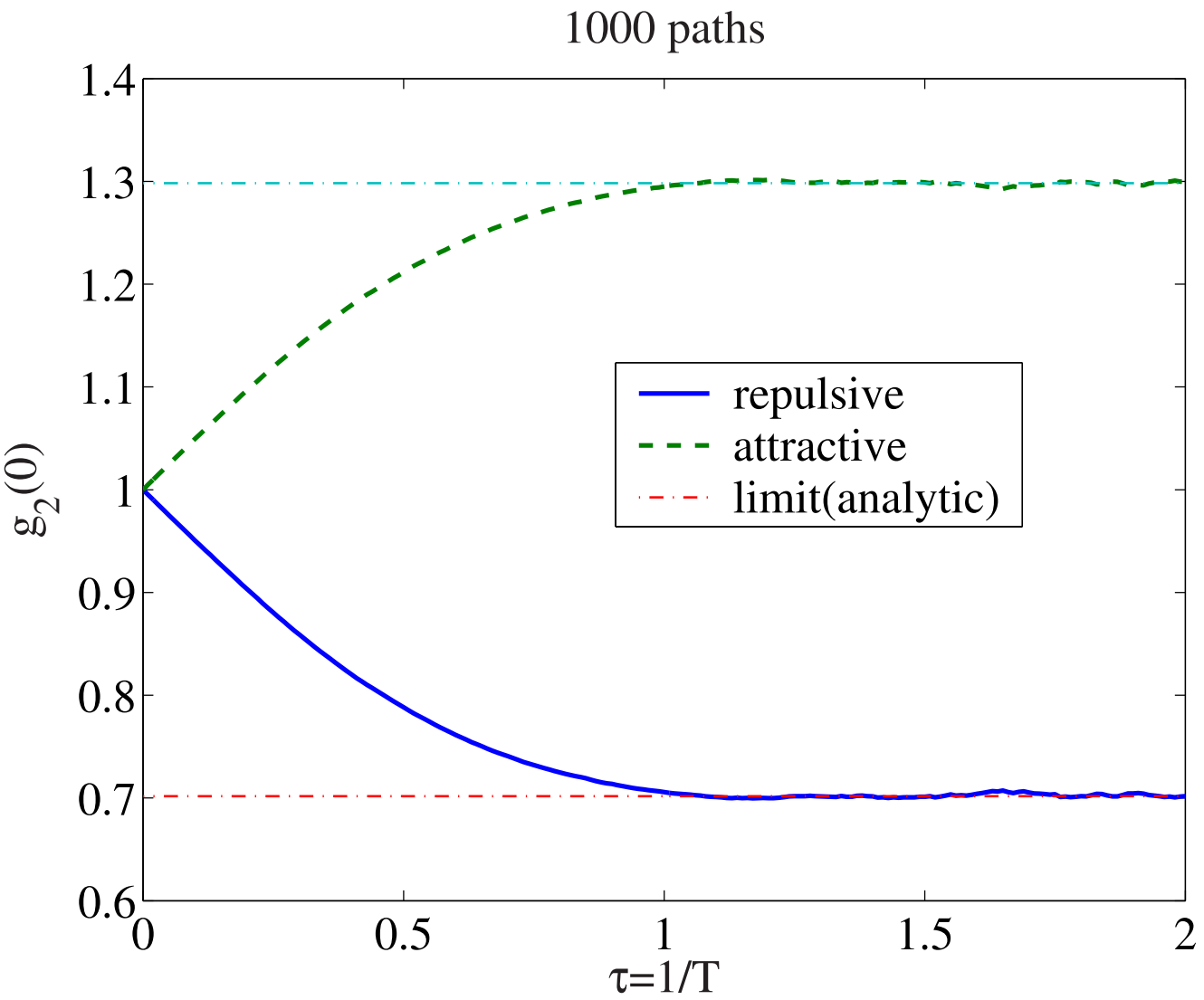
$$\frac{d\mathbf{n}_\sigma}{d\tau} = -\frac{1}{2}\left\{(\mathbf{I}-\mathbf{n}_\sigma)\,\Delta_\sigma^{(1)}\mathbf{n}_\sigma + \mathbf{n}_\sigma\Delta_\sigma^{(2)}\,(\mathbf{I}-\mathbf{n}_\sigma)\right\},$$

where the stochastic propagator matrix is

$$\Delta^{(r)}_{i,j,\sigma} = \left[-t_{ij} + \delta_{i,j}\left\{Un_{jj,\sigma'} - |U|n_{jj,\sigma} + \frac{1}{2}|U| - \mu\right\}\right] \pm \delta_{ij}\sqrt{2|U|}\xi^{(r)}_j$$

- $\xi^{(r)}_j$ are delta-correlated white noises

1D Lattice-100 sites



Branching

- averages are weighted,eg

$$\left\langle \widehat{\mathbf{n}}(\tau) \right\rangle = \frac{\sum_{j=1}^{N_p} \Omega^{(j)}(\tau) \mathbf{n}^{(j)}(\tau)}{\sum_{j=1}^{N_p} \Omega^{(j)}(\tau)}$$

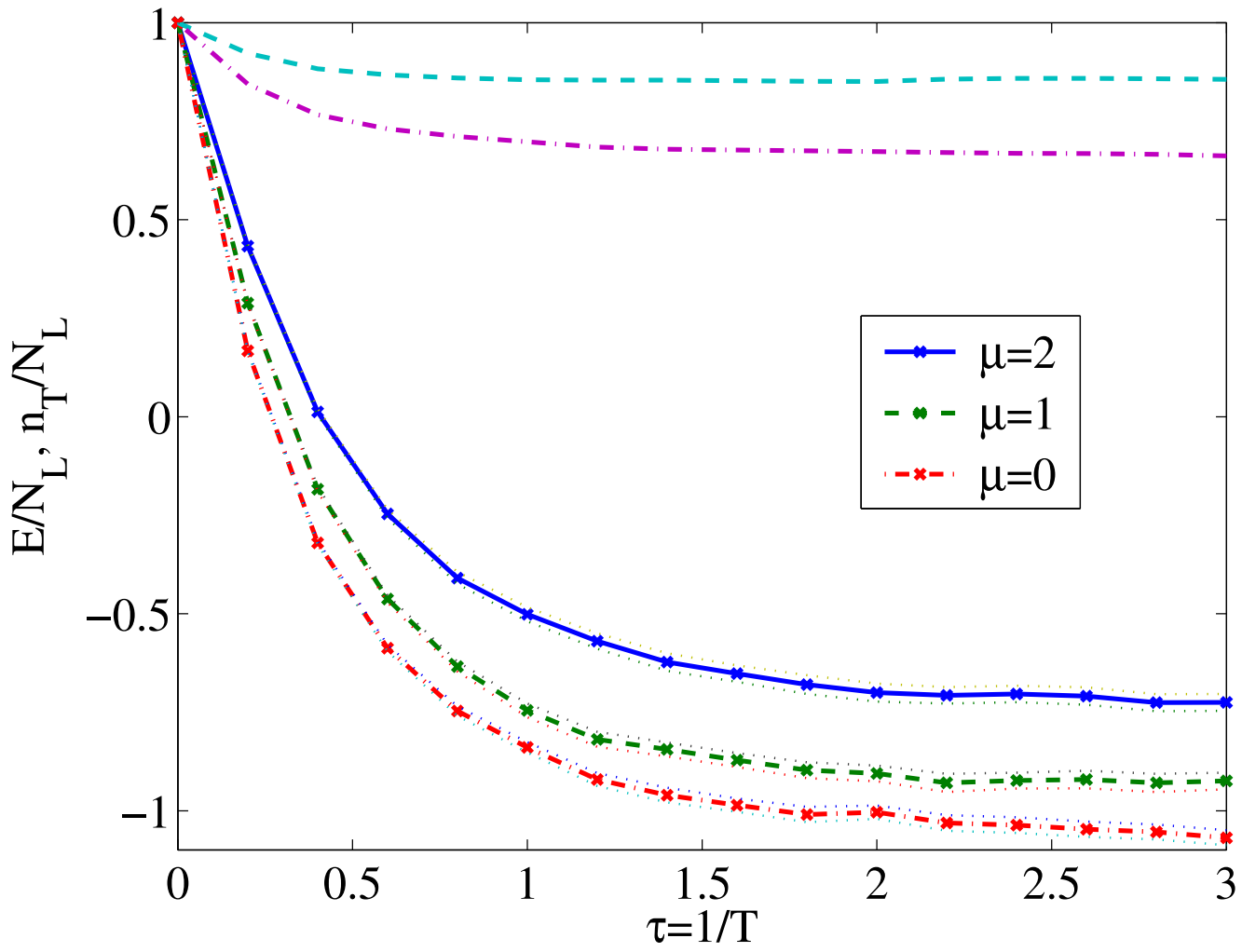
✘ but weights spread exponentially $\Longrightarrow$ many irrelevant paths

$\Longrightarrow$ delete low-weight paths and clone high-weight paths:

$$m^{(jp)} = \text{Integer}\left[\xi + \Omega^{(jp)}/\overline{\Omega}\right]$$

- $\xi \in [0,1]$ is a random variable, $\overline{\Omega}$ is an average weight
- after branching, weights of surviving paths are equalised

16x16 2D Lattice



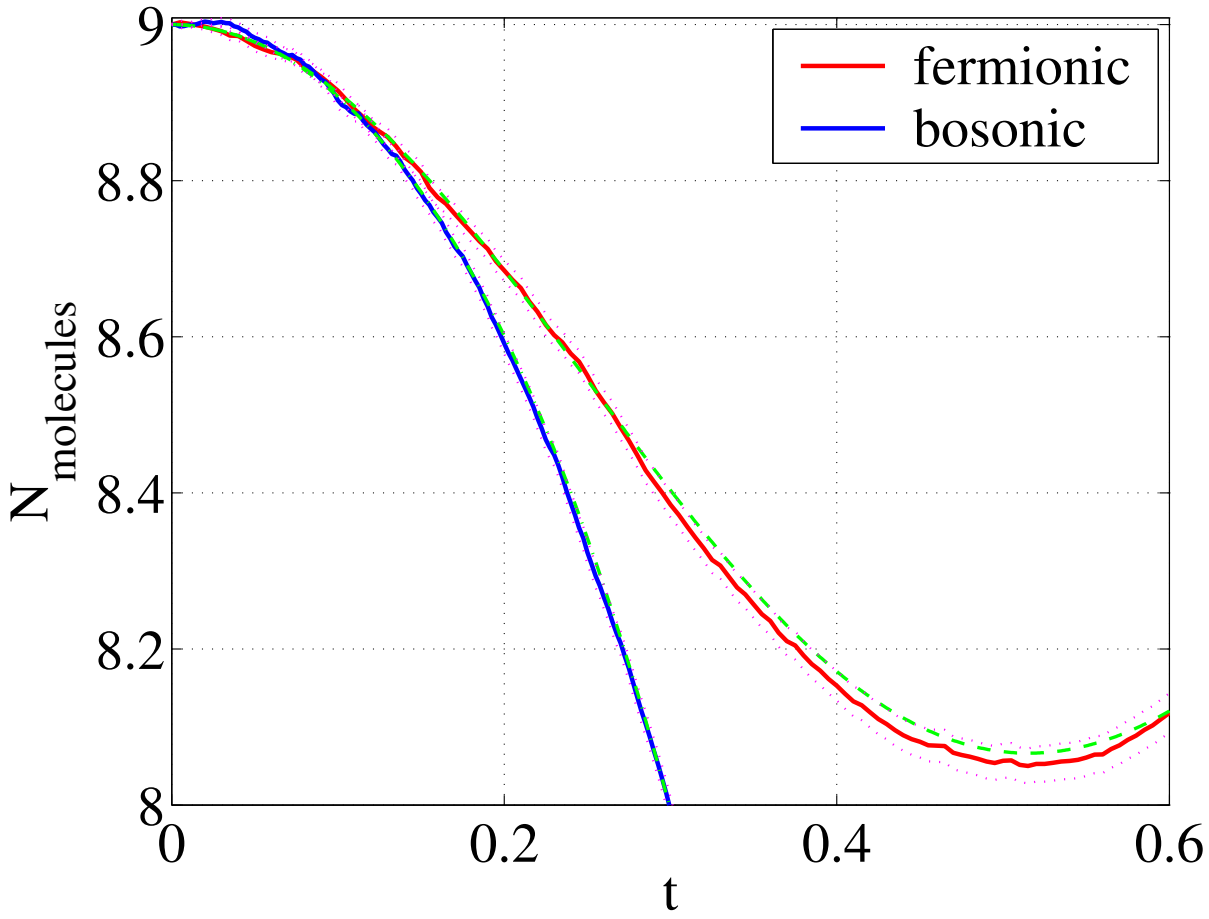
❄ *No sign problem!*

Application III: Molecules in a well

❄ Hamiltonian: $\widehat{H} = \widehat{a}\widehat{b}_1^{\dagger}\widehat{b}_2^{\dagger} + \widehat{a}^{\dagger}\widehat{b}_1\widehat{b}_2$

$$
\begin{aligned}
\dot{n}_1 &= i\chi(\alpha^{+}m - \alpha m^{+}) \pm \sqrt{i\chi}n_1\left(m\zeta_1^{*} + m^{+}\zeta_2^{*}\right) , \\
\dot{n}_2 &= i\chi(\alpha^{+}m - \alpha m^{+}) \pm \sqrt{i\chi}n_2\left(m\zeta_1^{*} + m^{+}\zeta_2^{*}\right) , \\
\dot{m} &= -i\chi\alpha(1 \pm n_1 \pm n_2) + \sqrt{i\chi}\left(\pm m^2\zeta_1^{*} + n_1n_2\zeta_2^{*}\right) , \\
\dot{m^{+}} &= i\chi\alpha^{+}(1 \pm n_1 \pm n_2) + \sqrt{i\chi}\left(n_1n_2\zeta_1^{*} \pm m^{+2}\zeta_2^{*}\right) , \\
\dot{\alpha} &= -i\chi m - \sqrt{i\chi}\zeta_1 , \\
\dot{\alpha^{+}} &= i\chi m^{+} + \sqrt{i\chi}\zeta_2 ,
\end{aligned}
$$

Result: Pauli blocking



Summary

- Generalised phase-space representations provide a means of simulating many-body quantum physics from first principles, with *precision limited only by sampling error*.

- Coherent-state-based methods have been successful in simulating quantum dynamics of photons and weakly interacting ultracold gases.

- Gaussian-based methods extend the applicability to highly correlated sysems of bosons and *fermions*.

- Simulated the Hubbard model (fermions in a lattice) *without sign errors*.