# From quantum fields to ecosystems

## Dynamics on extended phase-spaces

P. D. Drummond

ACQAO COE, University of Queensland

Moyal medal lecture, 2007

# Outline

1. Exponential complexity
   - Many-body systems
   - Classical phase-space

2. Extended phase-space
   - Quantum theory: +P and friends
   - Genetics on phase-space

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ULTRALOW temperatures down to $1nK$

TESTS QUANTUM THEORY IN NEW REGIMES!

- Bose-Einstein condensates: atom 'photons'
- Atom lasers, atomic diffraction, interferometers..
- Quantum superfluid fermions: atom 'electrons'
- Universality: Strongly interacting fermions
- Superchemistry: Stimulated molecule formation
- Color Superfluids: Multi-species fermi gases

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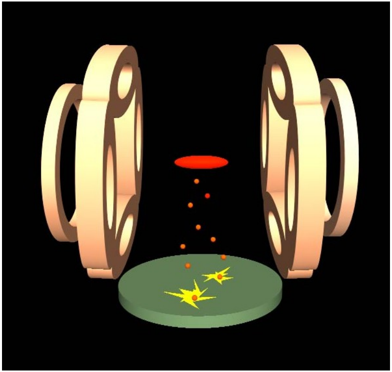
# Typical experiment (Orsay, ANU)



# Problem: quantum theory is exponentially complex!

Quantum many-body states are too large to store.

- consider $n$ particles distributed among $m$ modes
  - take $n \simeq m \simeq 500,000$:
  - Number of quantum states: $N_s = 2^{2n} = 2^{1,000,000}$
- More basis states than atoms in the universe
- Can't caculate with a $2^{1,000,000} \times 2^{1,000,000}$ matrix!

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  **intractable for $\gtrsim 5$ particles**
- operator factorization
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- perturbation theory
  **diverges at strong couplings**
- exact solutions
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- rate equation method
  **ignores fluctuations**
- quasi-species theory
  **not applicable to population dynamics**
- 'brute force' matrix method
  **only works for small genetic diversity and populations**
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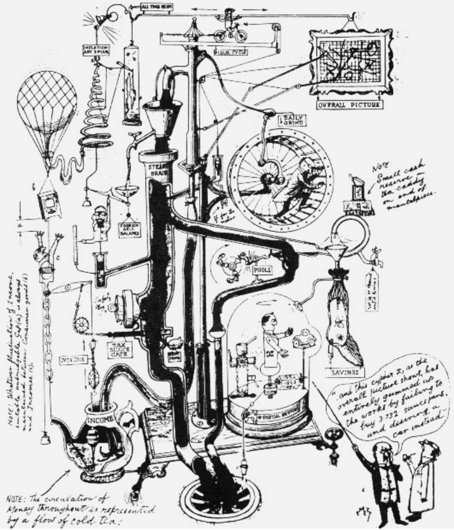
# Dedicated, special purpose computers?




**This computer solves the problems of economics: a Howard/Rudd Xmas present!**

Special-purpose computers have been proposed to solve exponential complexity. These include quantum computers, DNA computers, and adiabatic computers.

Problem:
still under development.

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# Quantum theory in Wigner/Moyal phase-space

$$\widehat{\rho} = \int P(\alpha)\hat{\Lambda}(\alpha)d^2\alpha$$

## Properties of Wigner/Moyal phase-space

- Maps quantum states into classical phase-space $\alpha = p + ix$
- **Wigner published the idea in statistical mechanics**
- Moyal: **theory is equivalent to quantum mechanics**
- Advantage: complexity grows linearly with mode number!

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# Moyal arriving at ANU

# Classical phase-space time-evolution

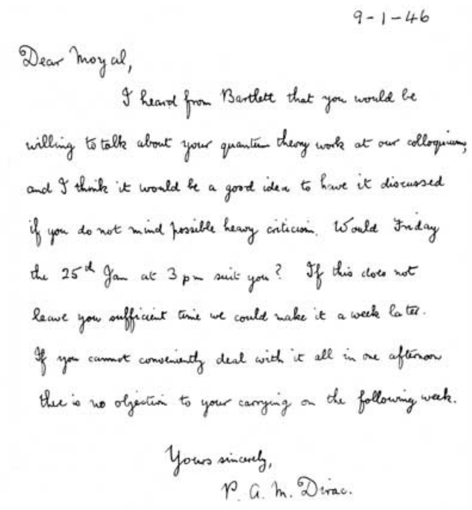
**Moyal showed how to calculate time-evolution!**

- Moyal brackets map quantum operators to differential equations
- **Famous correspondence with Dirac (who initially prevented publication)**
- Widely used in many areas of physics and elsewhere

**Dirac's criticism:** ***probabilities can't have negative values***

- **Later work of Husimi, Glauber, Sudarshan, Agarwal, Lax.**

# Classical phase-space time-evolution

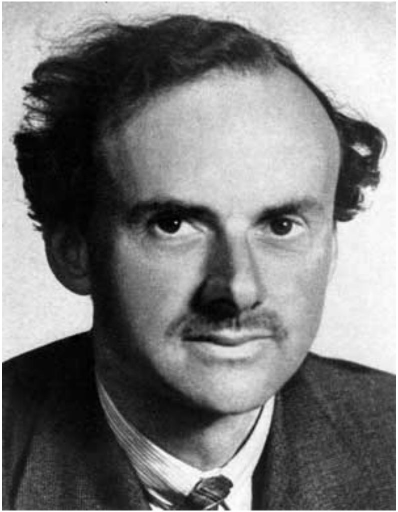


9-1-46

Dear Moyal,

I heard from Bartlett that you would be willing to talk about your quantum theory work at our colloquium, and I think it would be a good idea to have it discussed if you do not mind possible heavy criticism. Would Friday the 25th Jan at 3 pm suit you? If this does not leave you sufficient time we could make it a week later. If you cannot conveniently deal with it all in one afternoon there is no objection to your carrying on the following week.

Yours sincerely,
P. A. M. Dirac.



# Coherence theory, lasers and phase-space


## 2005 Nobel Prize in Physics

- one half to **Roy J. Glauber**
  - ***for his contribution to the quantum theory of optical coherence***
- one half to **Ted Haensch** and **Jan Hall**
  - **for their contributions to the the development of laser-based precision spectroscopy**

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# +P PHASE-SPACE METHODS

$$\widehat{\rho} = \int P(\alpha,\beta)\frac{|\alpha\rangle\langle\beta|}{\langle\beta||\alpha\rangle}d^2\alpha d^2\beta$$

**Enlarged** phase-space allows positive probabilities!

- Maps quantum states into 4M real coordinates: $\alpha,\beta = p+ix, p'+ix'$
- **A positive distribution always exists**
- Advantage: Time-evolution obeys a diffusion equation!
- Maps into a stochastic equation which can be randomly sampled

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# General phase-space approach

$$\widehat{\rho} = \int P(\overrightarrow{\lambda})\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda}$$

## Phase-space may be larger still!

- Here $\widehat{\Lambda}(\overrightarrow{\lambda})$ must be complete
- Quantum dynamics $\rightarrow$ Trajectories in $\overrightarrow{\lambda}$.
- Different basis choice $\widehat{\Lambda}(\overrightarrow{\lambda}) \rightarrow$ different representation
- Eg, positive P-representation: $\widehat{\Lambda}(\overrightarrow{\lambda}) = |\alpha\rangle\langle\beta| / \langle\beta||\alpha\rangle$

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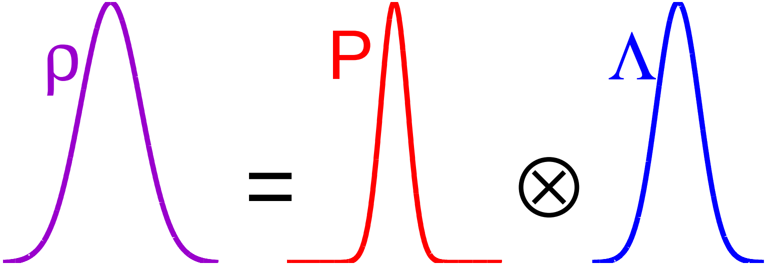
# Trade-offs: distribution vs basis




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

# Gaussian operator

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

**Quantum phase-space:** $\overrightarrow{\lambda} = (\Omega, \underline{\alpha}, \underline{\underline{\sigma}})$.

- Exponential of a quadratic form in the mode operator $\delta\underline{\widehat{a}} = (\widehat{\mathbf{a}}, \widehat{\mathbf{a}}^{\dagger}) - \underline{\alpha}$ ,
- $\underline{\alpha}$ is a mean displacement
- $\widehat{\mathbf{a}}$ is the vector of mode operators
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# Stochastic gauge equations

$$d\Omega/\partial t = \Omega[U + \mathbf{g}\cdot\boldsymbol{\zeta}]$$
$$d\boldsymbol{\alpha}/\partial t = \mathbf{A} + \mathbf{B}(\boldsymbol{\zeta} - \mathbf{g})$$

**Exponential quantum problems → tractable stochastic equations**

- Can be used for fermions AND bosons
- Many trajectories needed to control growing sampling errors
- $\mathbf{g}$ is a gauge chosen to stabilize trajectories
- Careful choice of basis, gauge and stochastic method!

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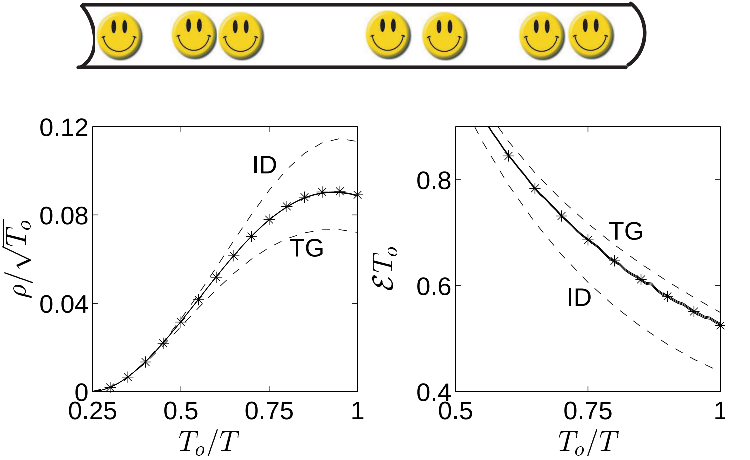
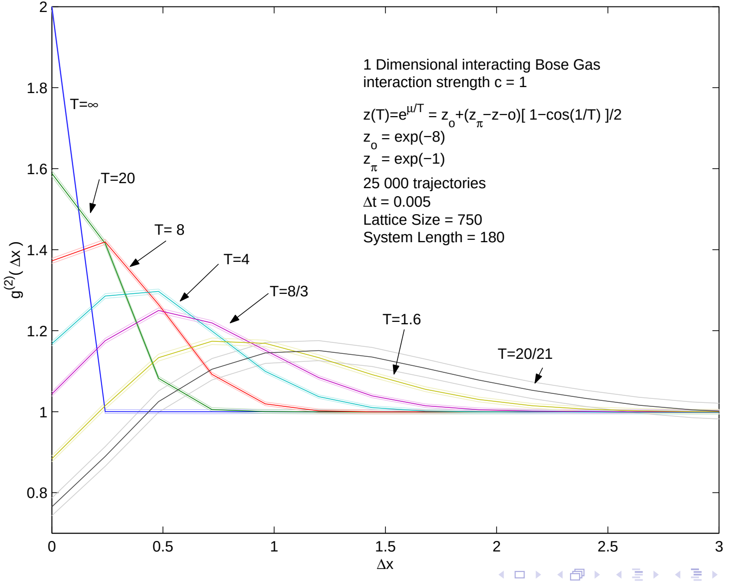
# ONE-DIMENSIONAL BEC




*Agreement of simulations with exact solutions*

# Predicts: anomalous spatial correlations



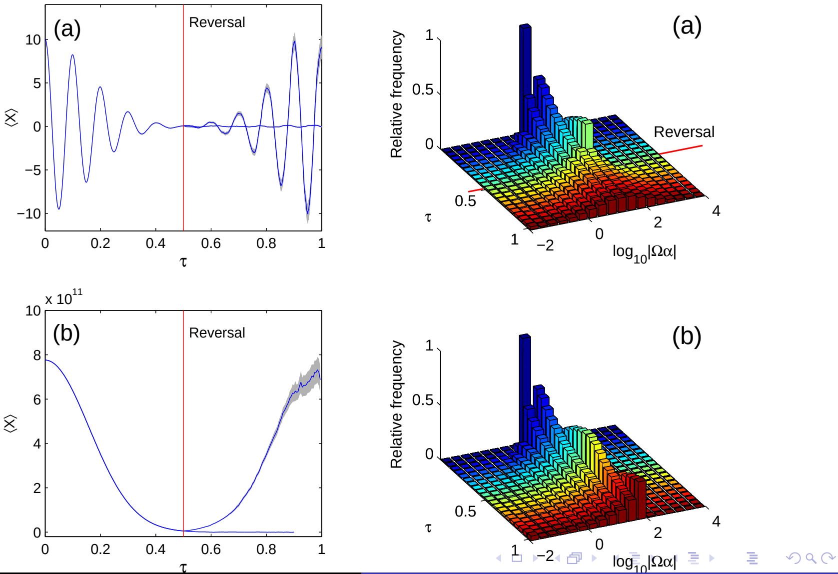
# BEC QUANTUM DYNAMICS, SINGLE WELL (BLOCH)

**Single-mode case:**

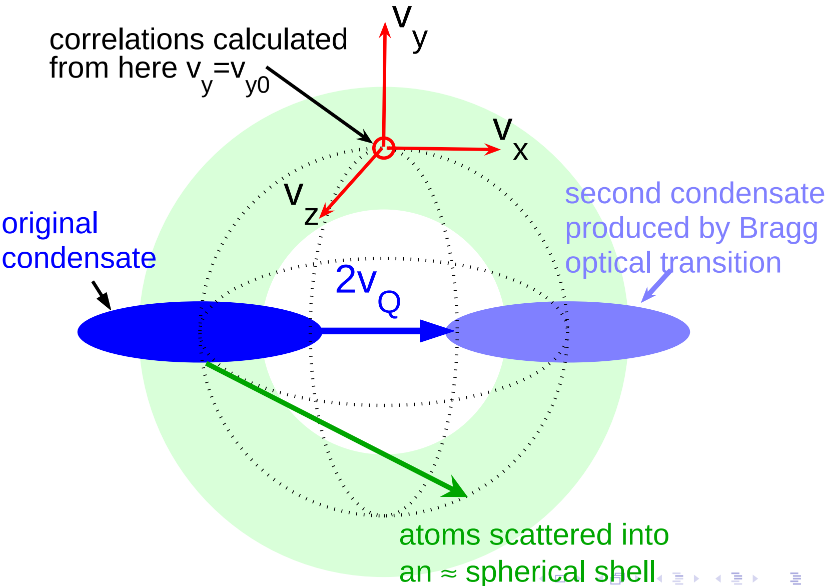
$$
\begin{aligned}
i\frac{d\alpha}{d\tau} &= \left[|\alpha\beta^*| + \omega + \sqrt{i}\zeta_1(\tau)\right]\alpha \\
i\frac{d\beta}{d\tau} &= \left[|\alpha\beta^*| + \omega + \sqrt{i}\zeta_2(\tau)\right]\beta \\
\frac{d\Omega}{d\tau} &= \Omega g_i \zeta_i(\tau)
\end{aligned}
$$

- Unitary evolution of $10^{23}$ interacting bosons

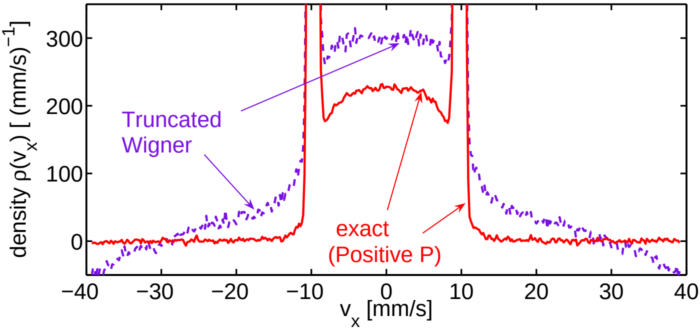
# Time-reversal test of unitary evolution



# BEC collision of 150,000 atoms (Ketterle, Aspect)



# Positive-P vs Truncated Wigner Moyal




**Quantum collisions of 150,000 atoms, two million modes - Phys Rev Letts Editors Award, 2007**

# Outline

# Why *simulate genetics using physics tools?*

The goal of theoretical science is to make testable predictions.

***Central problem of modern theoretical biology!***

- Gene sequencing now can generate data on a scale rivalling any physics experiment
- Populations of micro-organisms - like viruses - evolve rapidly, and involve numbers of order $10^9$ or more.
- How can we model the evolution of large natural populations with enormous genotype variation?

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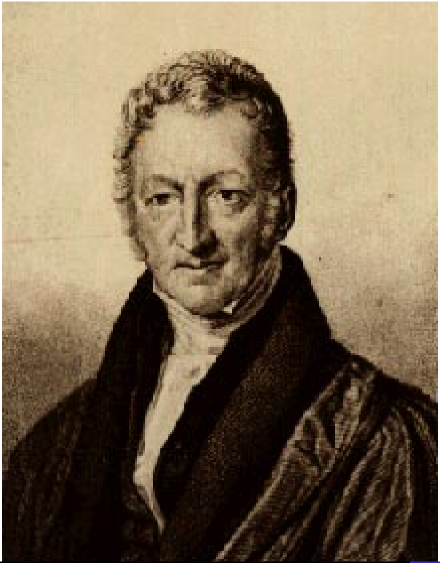
# POPULATION DYNAMICS



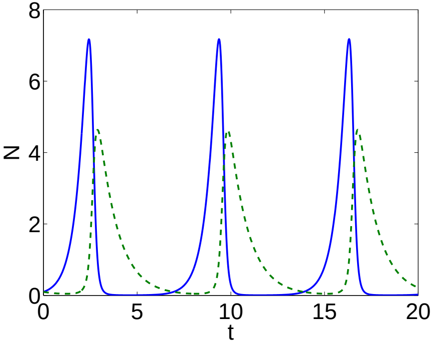
Malthus (1798) developed the model of exponential population growth.

$$\dot{N} = gN$$

Refined by Verhulst (1838) to give the logistic equation:

$$\dot{N} = gN - kN^2$$

# Predator-Prey dynamics: Lotka-Volterra



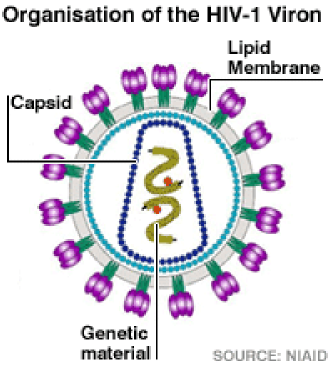

Prey (solid line)

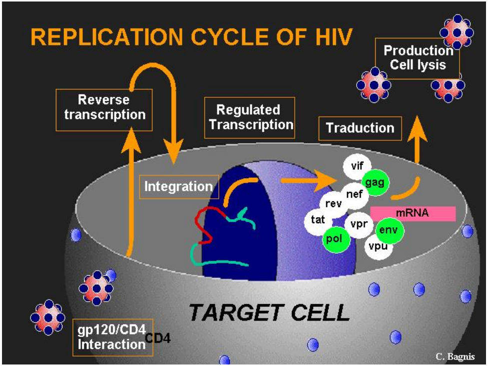
$$\dot{N}_1 = N_1 \left( G_1 - C_{12} N_2 \right)$$

Predator (dotted line):

$$\dot{N}_2 = -N_2 \left( G_2 - C_{12} N_1 \right)$$

# Human HIV virus lifecycle:



# Viral infection models

$$\frac{\partial N_1}{\partial t} = S_1 + N_1 G_1 - C_{12} N_1 N_2 \qquad \textit{Uninfected cells}$$

$$\frac{\partial N_2}{\partial t} = G_{23} N_3 + N_2 G_2 - C_{12} N_1 N_2 \qquad \textit{Free viruses}$$

$$\frac{\partial N_3}{\partial t} = N_3 G_3 + C_{21} N_1 N_2 \qquad \textit{Infected cells}$$

# MUTATION

Natural populations are heterogenous and stochastic!

## There is enormous genetic variety everywhere!

- Even simple reproduction is a random event
- Rapid mutation occurs with RNA viruses
- Interactions mean that growth is NOT independent
- $N^M$ possibilities, for $M = 4^B$ mutations over $B$ bases.

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# RNA Viruses

- HIV, Ebola, SARS, Influenza, Dengue, Hepatitis C .
- Gene: ribonucleic acid (RNA), $\sim 10^4$ nucleotide bases
- RNA viruses have very high mutation rates:
- HIV: $\sim 10^9$ - $10^{10}$ virions every day, per person,
  - $3 \times 10^{-5}$ mutations per nucleotide per replication cycle
  - $6 \times 10^6$ **new infections/ year,** $3 \times 10^6$ **deaths**

# Stochastic Genetics

FIsher (1930) introduced the idea of genetic correlations and probability in analysing inherited characteristics.

# Poisson Representation

- Master Equation: $\frac{d}{dt}P(\mathbf{N}) = \sum_{\mathbf{N}'} \mathscr{M}_{\mathbf{N}\mathbf{N}'} P(\mathbf{N}')$
- Poisson Expansion: $P(\mathbf{N}) = \int d[\vec{\alpha}]\, f(\vec{\alpha})\, P(\mathbf{N};\vec{\alpha})$ ,
- Here $P(\mathbf{N}|\vec{\alpha})$ is the Poisson distribution, with:

$$P(\mathbf{N};\vec{\alpha}) = \Omega \prod_i \frac{e^{-\alpha_i} (\alpha_i)^{N_i}}{N_i!} .$$

# Genetic phase-space equations

Consider the most general kinetic equation, which is:

$$\varepsilon_1 X_1 + \varepsilon_2 X_2 \overset{G}{\longrightarrow} \varepsilon_3 X_3 + \varepsilon_4 X_4$$

Equivalent Fokker-Planck equation (where $\partial_i = \partial / \partial \alpha_i$):

$$\frac{df}{dt} = \mathscr{L} f = G \left[ (1-\partial_3)^{\varepsilon_3} (1-\partial_4)^{\varepsilon_4} - (1-\partial_1)^{\varepsilon_1} (1-\partial_2)^{\varepsilon_2} \right] \alpha_1^{\varepsilon_1} \alpha_2^{\varepsilon_2} f$$

# Random birth, death, mutation

Need to calculate the time-evolution of probabilities $P(\mathbf{N})$, for finding the total number of individuals of each type equal to $\mathbf{N} = (N_1, .., N_d)$, for

$$X_i \quad \overset{G^B_{ji}}{\longrightarrow} \quad X_i + X_j \, ,$$

$$X_i \quad \overset{\phi_i}{\longrightarrow} \quad 0 \, .$$

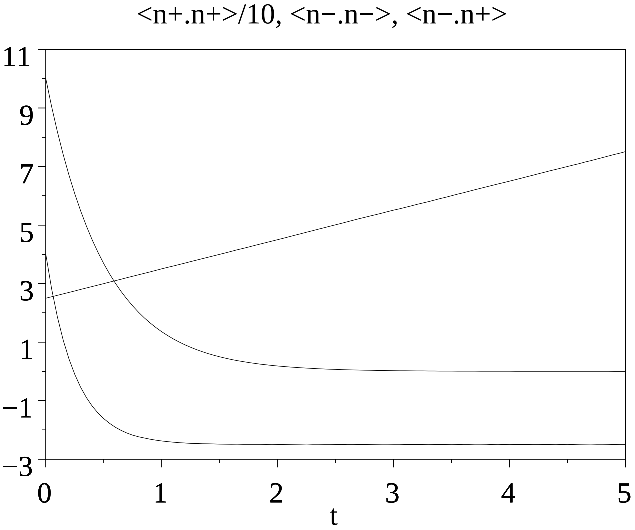
# Two-species case: exact stochastic equations

Suppose that mutations always occur, so $G_{11}^B = G_{22}^B = 0$, and it is symmetric, so $G_{12}^B = G_{21}^B = k_m$. This can be simplified further, on introducing $n^{\pm} = (\alpha_1 \pm \alpha_2)$:

$$\frac{dn^+}{dt} = (k_m - \phi)n^+ + \sqrt{2k_m n^+}\zeta_1(t)$$

$$\frac{dn^-}{dt} = -(k_m + \phi)n^- + i\sqrt{2k_m n^+}\zeta_2(t)\,.$$

# Simulated vs Exact Correlations - indistinguishable!



# SUMMARY

Phase-space representation methods have many applications

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- Maps **quantum field evolution** into a stochastic equation
- Can also be used to treat genetics and population dynamics
- Advantage: No exponential complexity issues!
- **'Best available method for strongly-interacting fermions'**
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