

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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Ultracold atoms - the ideal quantum system

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

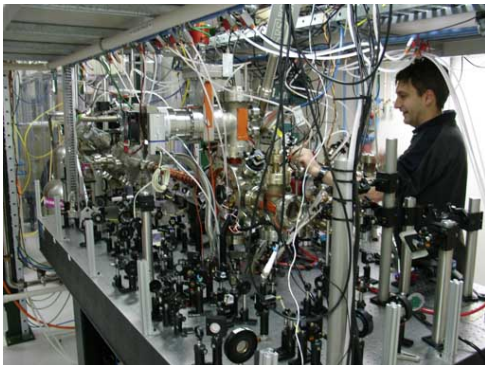
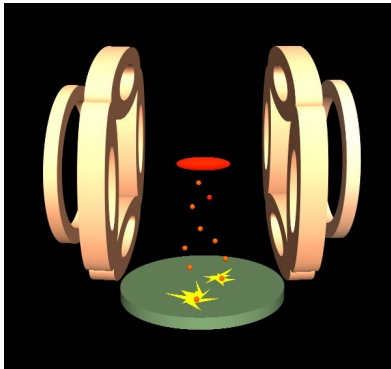
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Typical experiment (Orsay, ANU)



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 calculate with a $2^{1,000,000} \times 2^{1,000,000}$ matrix!**

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- operator factorization
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- consider n individuals distributed among m genotypes
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Traditional bio-informatics and ecosystem methods?

- 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
- Monte-Carlo (Gillespie technique)
very slow for large populations

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Quantum theory in Wigner/Moyal phase-space

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

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.

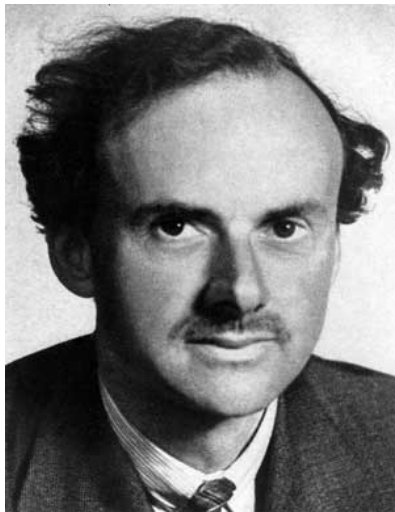
Classical phase-space time-evolution

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 development of laser-based precision spectroscopy**

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+P PHASE-SPACE METHODS

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

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

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

Phase-space may be larger still!

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

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Trade-offs: distribution vs basis

$$\rho = P \otimes \Lambda$$
$$\sigma_\rho \sim \sigma_P + \sigma_\Lambda$$

Gaussian operator

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

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

- Exponential of a quadratic form in the mode operator $\delta \hat{\underline{a}} = (\hat{\underline{a}}, \hat{\underline{a}}^\dagger) - \underline{\alpha}$,
- $\underline{\alpha}$ is a mean displacement
- $\hat{\underline{a}}$ is the vector of mode operators
- treats either bosons (eg, photons) or fermions (eg, electrons)

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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 \rightarrow 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!

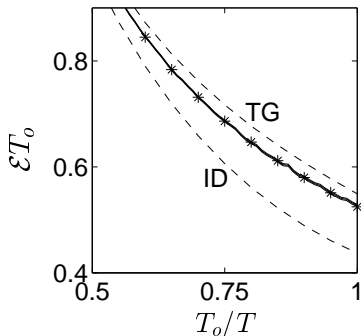
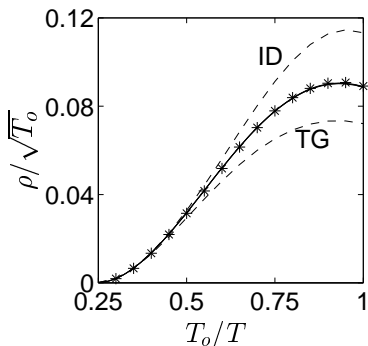
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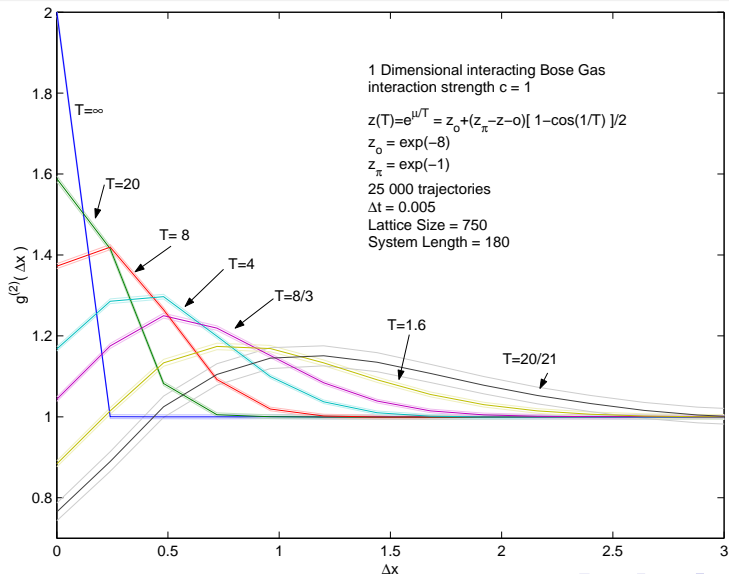
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ONE-DIMENSIONAL BEC



Agreement of simulations with exact solutions

Predicts: anomalous spatial correlations



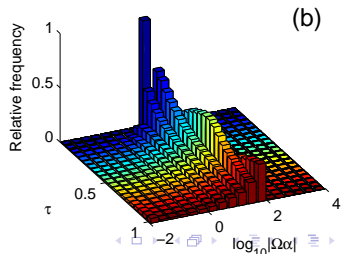
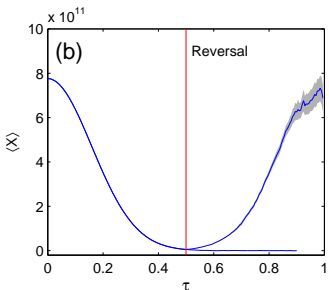
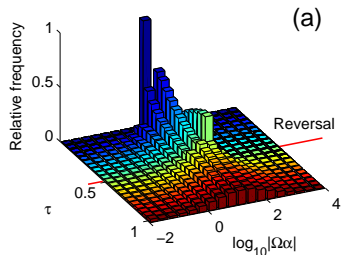
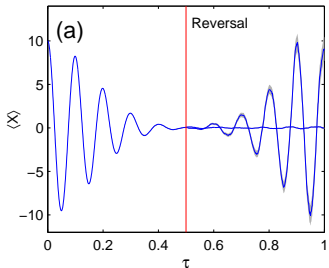
BEC QUANTUM DYNAMICS, SINGLE WELL (BLOCH)

Single-mode case:

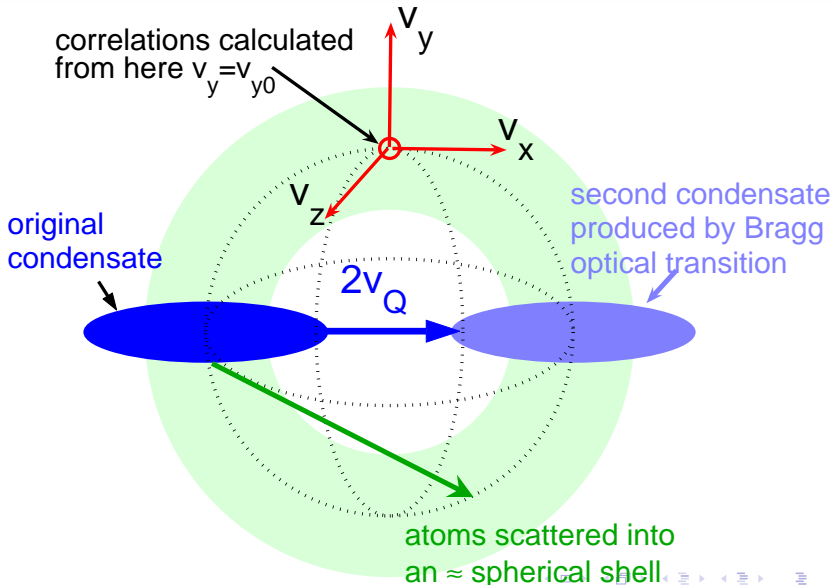
$$i \frac{d\alpha}{d\tau} = \left[|\alpha\beta^*| + \omega + \sqrt{i}\zeta_1(\tau) \right] \alpha$$
$$i \frac{d\beta}{d\tau} = \left[|\alpha\beta^*| + \omega + \sqrt{i}\zeta_2(\tau) \right] \beta$$
$$\frac{d\Omega}{d\tau} = \Omega g_i \zeta_i(\tau)$$

- Unitary evolution of 10^{23} interacting bosons

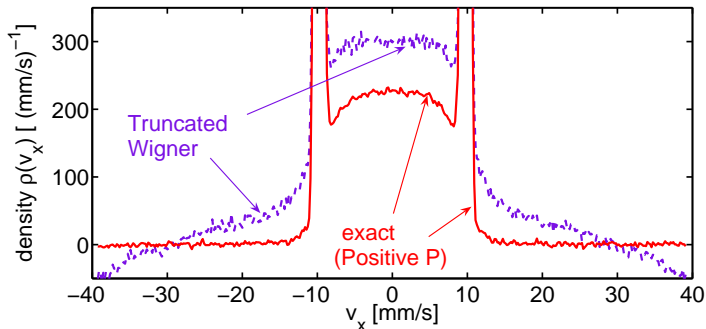
Time-reversal test of unitary evolution



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

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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



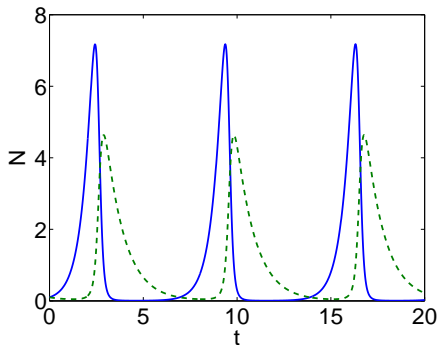
Malthus (1798) developed the model of exponential population growth.

$$\dot{N} = gN$$

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

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

Predator-Prey dynamics: Lotka-Volterra



Prey (solid line)

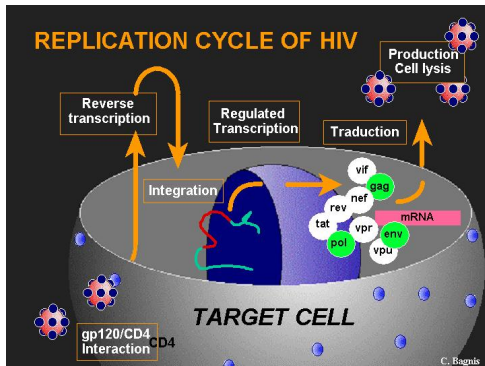
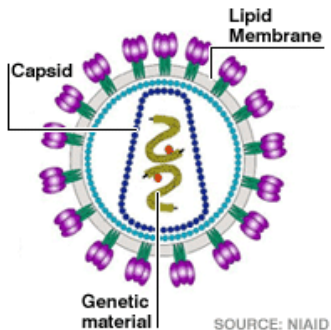
$$\dot{N}_1 = N_1 (G_1 - C_{12} N_2)$$

Predator (dotted line):

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

Human HIV virus lifecycle:

Organisation of the HIV-1 Viron



Viral infection models

$$\begin{aligned}\frac{\partial N_1}{\partial t} &= S_1 + N_1 G_1 - C_{12} N_1 N_2 && \textit{Uninfected cells} \\ \frac{\partial N_2}{\partial t} &= G_{23} N_3 + N_2 G_2 - C_{12} N_1 N_2 && \textit{Free viruses} \\ \frac{\partial N_3}{\partial t} &= N_3 G_3 + C_{21} N_1 N_2 && \textit{Infected cells}\end{aligned}$$

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,
 - 3×10^{-5} mutations per nucleotide per replication cycle
 - 6×10^6 new infections/ year, 3×10^6 deaths

Stochastic Genetics



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

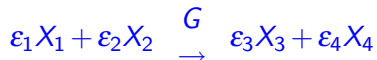
Poisson Representation

- Master Equation: $\frac{d}{dt}P(\mathbf{N}) = \sum_{\mathbf{N}'} \mathcal{M}_{\mathbf{N}\mathbf{N}'} P(\mathbf{N}')$
- 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:



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

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

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 $\mathbf{N} = (N_1, \dots, N_d)$, for

$$X_i \xrightarrow{G_{ji}^B} X_i + X_j,$$

$$X_i \xrightarrow{\phi_i} 0.$$

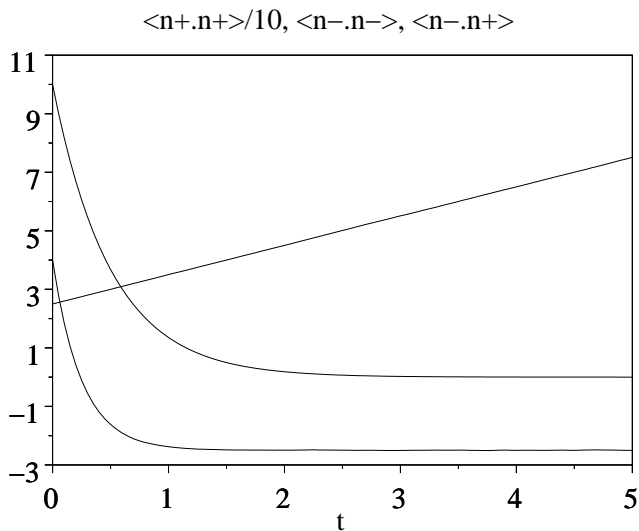
Two-species case: exact stochastic equations

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

Enlarged phase-space makes them true probabilities!

- 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'**
- Mathematical challenge:
 - sampling error often increases with time,
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