Quantum phase-space methods and the Fermi sign problem

Joel Corney and Peter Drummond

"Seek simplicity, and distrust it."
A. N. Whitehead (1861 – 1947)

J. F. Corney and P. D. Drummond, "Gaussian Quantum Monte Carlo methods for fermions and bosons", Phys. Rev. Lett. (to appear).

Why phase-space methods?

- Ultracold gases provide an elegant and well-controlled environment for exploring the fundamentals of quantum, many-body physics.
  - theoretical predictions can be tested precisely
  - need for first-principles calculations
- Phase-space methods can do this!

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M. K. Olsen, A. B. Melo, K. Dechoum and A. Z. Khoury, Phys. Rev. A 70, 043815 (2004).

M. R. Dowling, P. D. Drummond, M. J. Davis and P. Deuar

P. D. Drummond, P. Deuar, and K. V. Kheruntsyan, Phys. Rev. Lett. 92, 040405 (2004).

P.D. Drummond and P. Deuar, J. Opt. B: Quantum Semiclass. Opt. 5, S281-S289 (2003);

P. D. Drummond and J. F. Corney, Phys. Rev. A 60, R2661 (1999).

Fermions and antisymmetric complexity

- In QM, particles are indistinguishable:

$$P(x_1,x_2) = P(x_2,x_1)$$

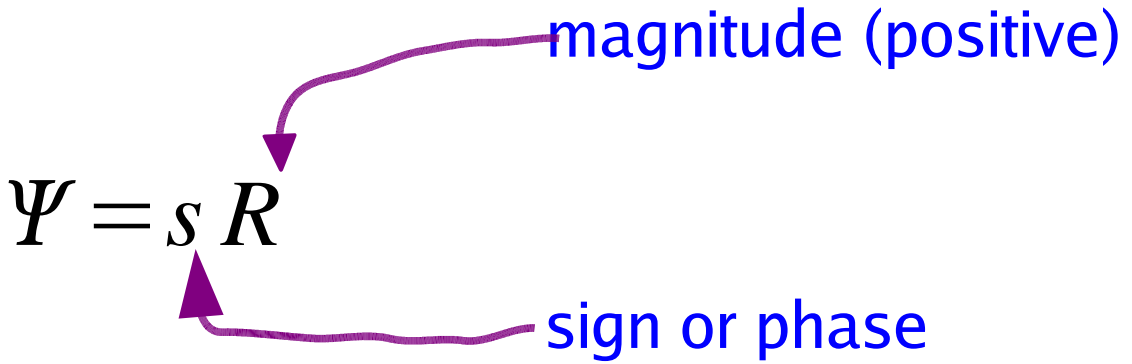
  - for bosons: $\psi(x_1,x_2) = \psi(x_2,x_1)$
  - for fermions: $\psi(x_1,x_2) = -\psi(x_2,x_1)$

- Nodal structure of antisymmetric wavefunction makes fermionic calculation much more difficult

Monte Carlo Methods

- treat wavefunction as a probability distribution
- use Monte Carlo methods to sample this multidimensional quantity

write



- for fermions, must keep track of sign

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W. von der Linden, "A quantum Monte-Carlo approach to many-body physics, Phys. Rep. 220, 53 (1992).

R. R. dos Santos, "Intro. to quantum Monte-Carlo simulations for fermionic systems," Braz. J. Physics 33, 36 (2003).

Fermion sign error

- physical quantities are weighted averages:

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

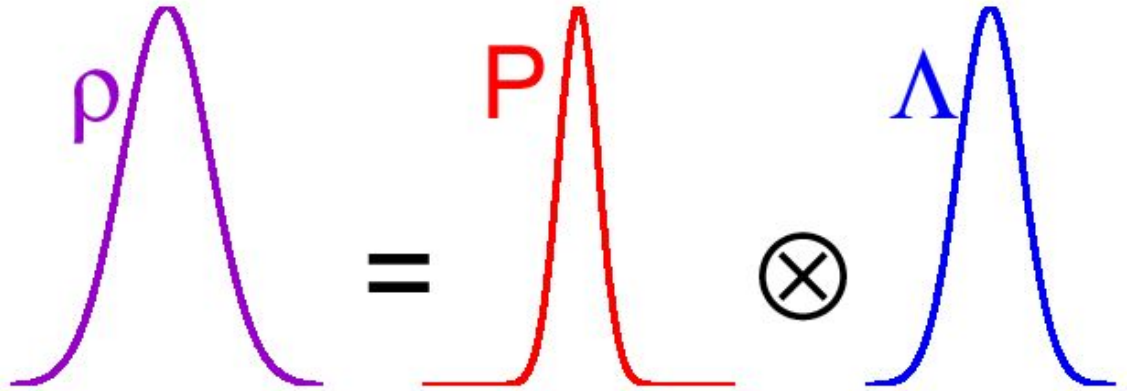
- as $\langle s \rangle \to 0$, sampling error gets bad

http://archive.ncsa.uiuc.edu/Science/CMP/lectures/signs.html
(google "sign problem")

- we can avoid this problem by sampling a distribution that is always positive

incorporate antisymmetric structure into the underlying basis

Phase-space representations



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

density operator

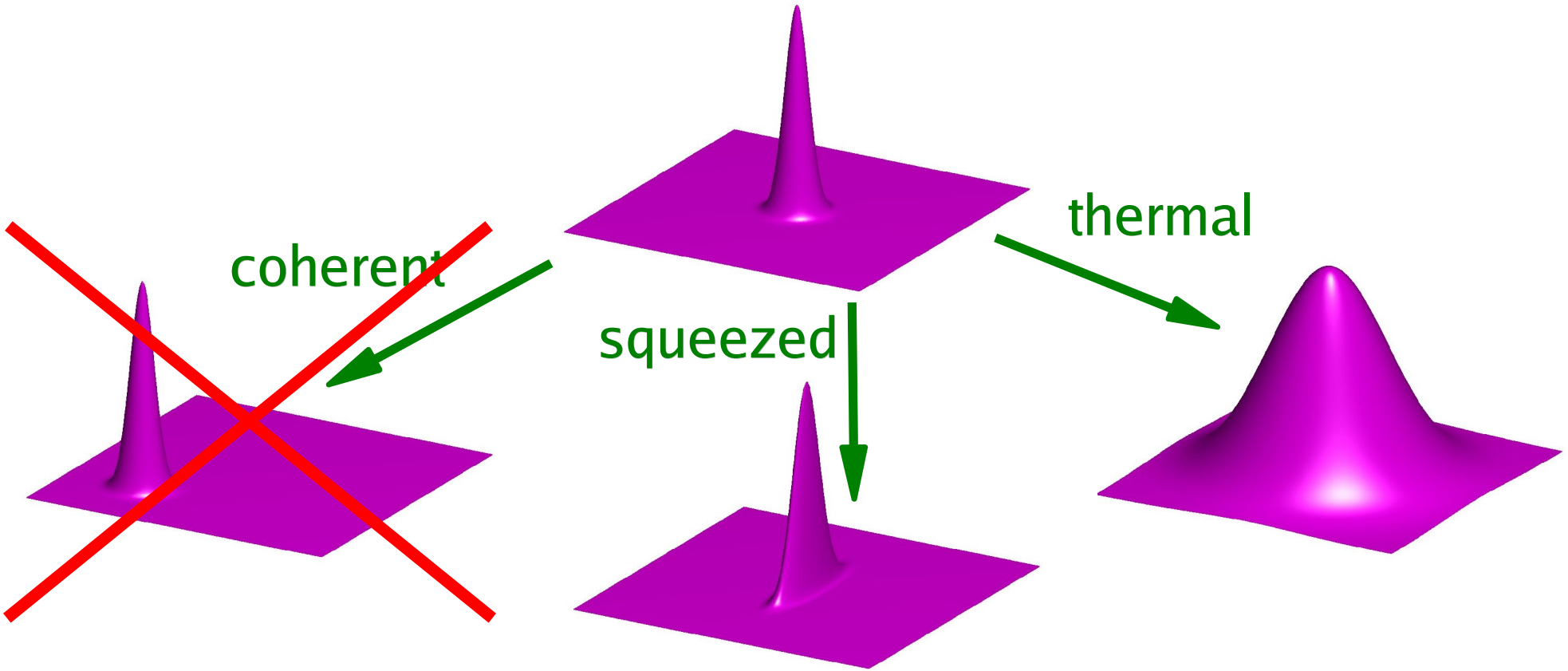
probability distribution

phase-space variables

operator basis

General Gaussian operators

a generalisation of the density operators
that describe Gaussian states

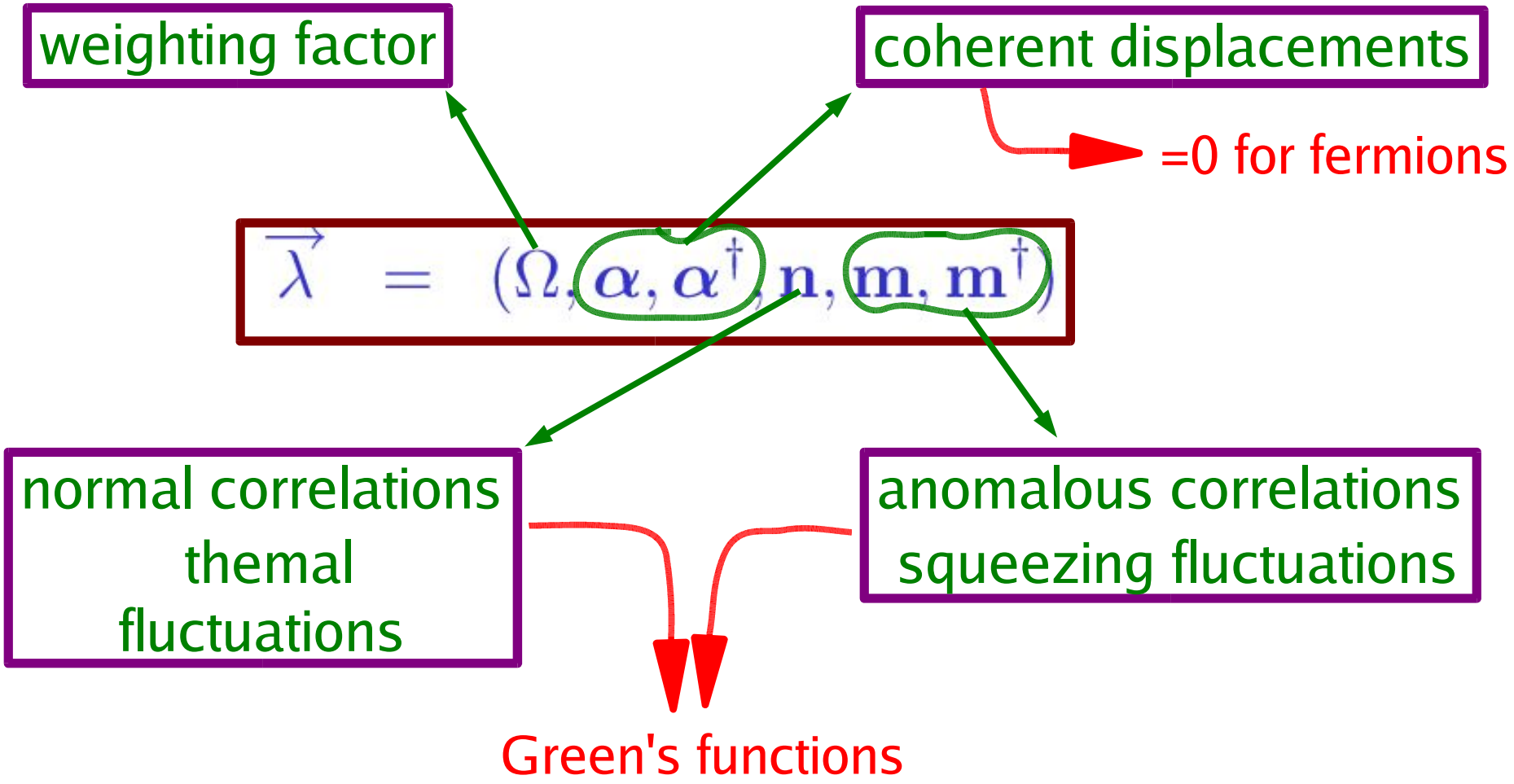


Why a general Gaussian basis?

- complete and positive representation of physical states
- no unphysical superpositions
  - obeys superselection rules
  - allows a natural phase-space method for fermions
- incorporates thermal and squeezed fluctuations (quasiparticles)
  - suited to ultracold quantum gases!

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

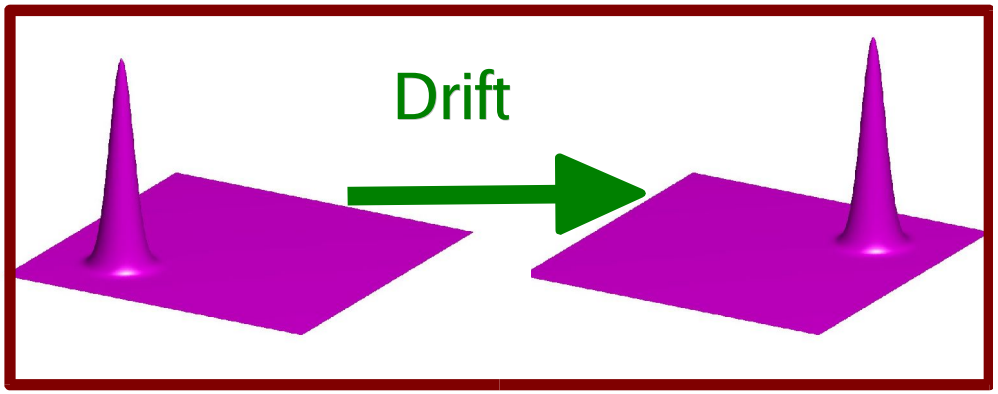
Extended phase space

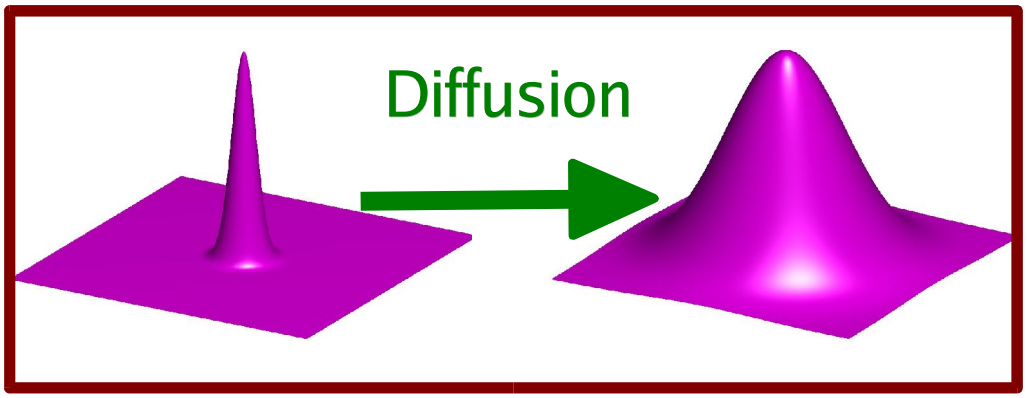


$$\widehat{\rho} = \int P(\vec{\lambda})\widehat{\Lambda}(\vec{\lambda})d\vec{\lambda}$$

Interacting many-body physics

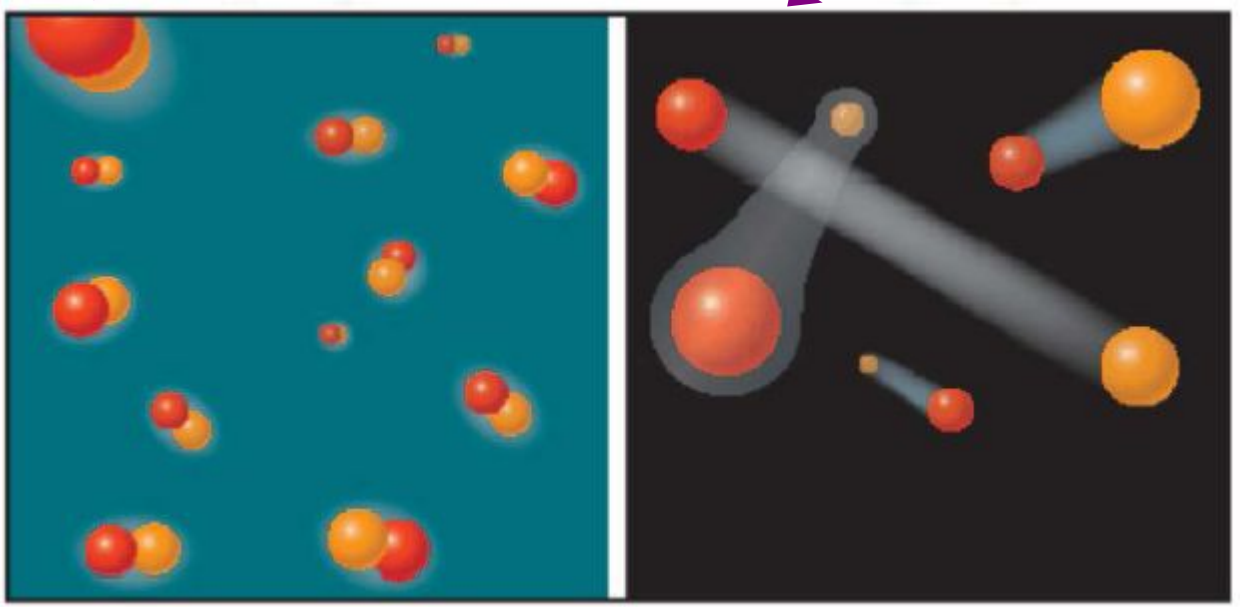
- many-body problems map to nonlinear stochastic equations
- calculations can be from first-principles
- precision limited only by sampling error
- adapt basis to suit the problem





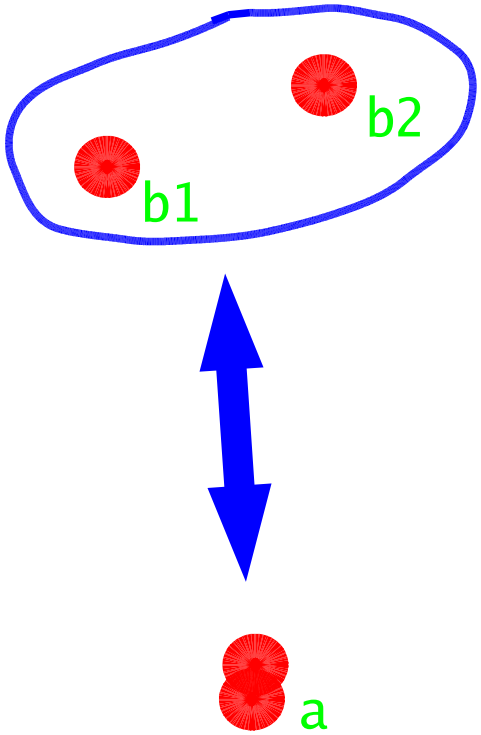
Molecule formation

- Coherently transfer atoms to bound states, using magnetic or optical fields
  - superchemistry for bosons
  - BEC to BCS crossover for fermions

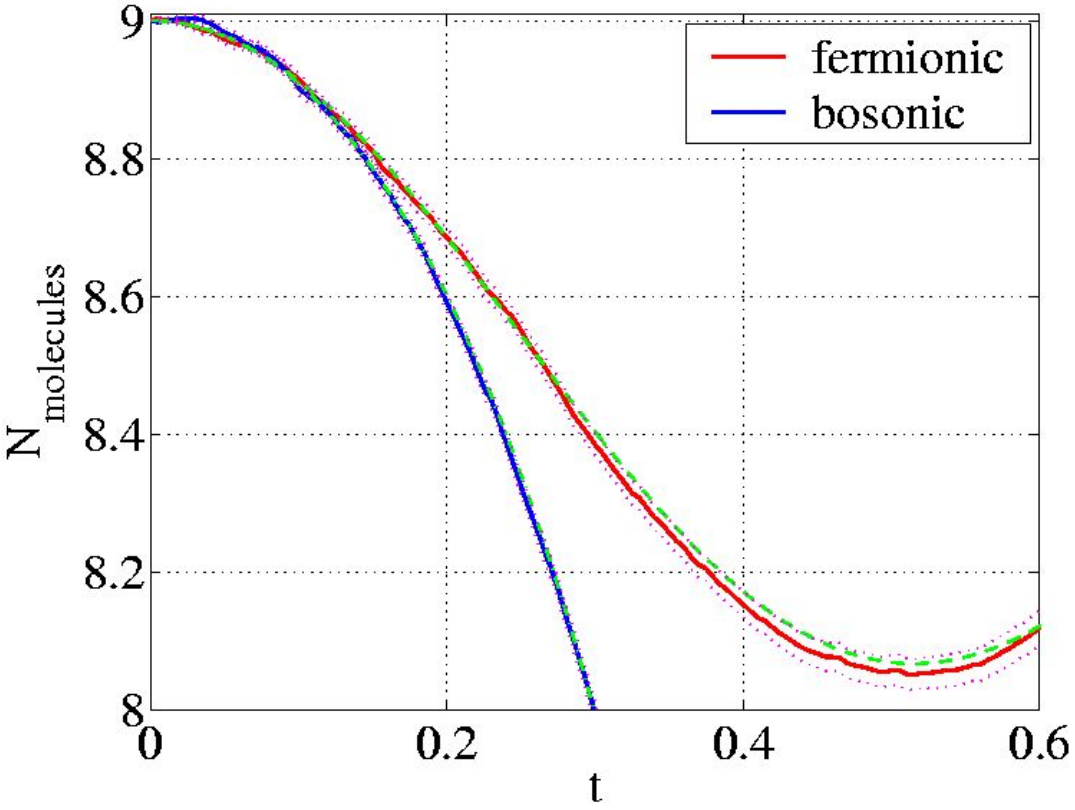


Atomic-molecular dynamics

$$\hat{H} = \hat{a}\hat{b}_1^\dagger\hat{b}_2^\dagger + \hat{a}^\dagger\hat{b}_1\hat{b}_2$$

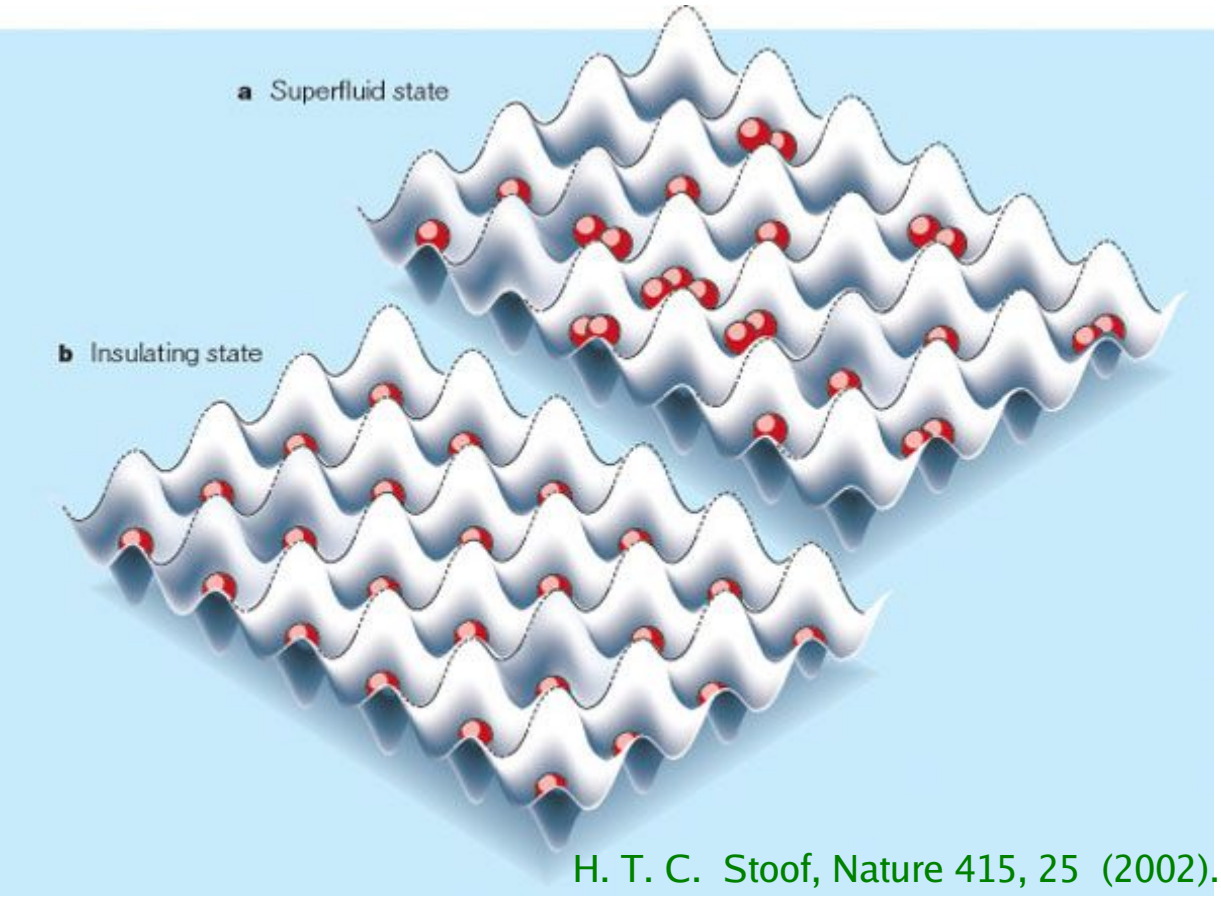


bosons
or
fermions



Pauli blocking for fermions

Cold atoms in a lattice



H. T. C. Stoof, Nature 415, 25 (2002).

- Bosons in a lattice described by Bose-Hubbard model
- Fermions in a lattice described by the Hubbard model

Hubbard model

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

interwell tunnelling

atomic interactions

- simplest model of an interacting Fermi gas on a lattice
- solid-state models; relevance to High-T_c superconductors
- only the 1D model is exactly solvable (Lieb & Wu, 1968)
- higher dimensions - use quantum Monte Carlo methods
- except for a few special symmetrical cases, QMC suffers from sign problems.
- errors increases with dimension, lattice size, interaction strength

Applying the Gaussian method (1 / 4)

- goal: solve the Grand canonical distribution:

$$\hat{\rho} = \exp(-(\hat{H} - \mu\hat{N})\tau)$$

unnormalised density operator

chemical potential

total number

scaled, inverse temperature $=1/k_B T$

- but this is impossible ! (except for $\tau = 0$)
- so rewrite as equation for temperature evolution:

$$\frac{d}{d\tau}\hat{\rho} = -\frac{1}{2}\left[(\hat{H} - \mu\hat{N})\hat{\rho} + \hat{\rho}(\hat{H} - \mu\hat{N})\right]$$

Applying the Gaussian method (2 / 4)

- apply mappings: *J. F. Corney and P. D. Drummond, cond-mat/0411712.*

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

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

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

  - Fokker-Planck equation for P
  - contains drift and diffusion
  - sample with stochastic equations

Applying the Gaussian method (3 / 4)

- How to get positive diffusion?
  - modify interaction term with a 'Fermi gauge':

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

  - get a positive-definite diffusion matrix
    - realise the diffusion with a real noise process
    - problem maps to a real (and much more stable) subspace

Applying the Gaussian method (4 / 4)

- final (Stratonovich) equations:

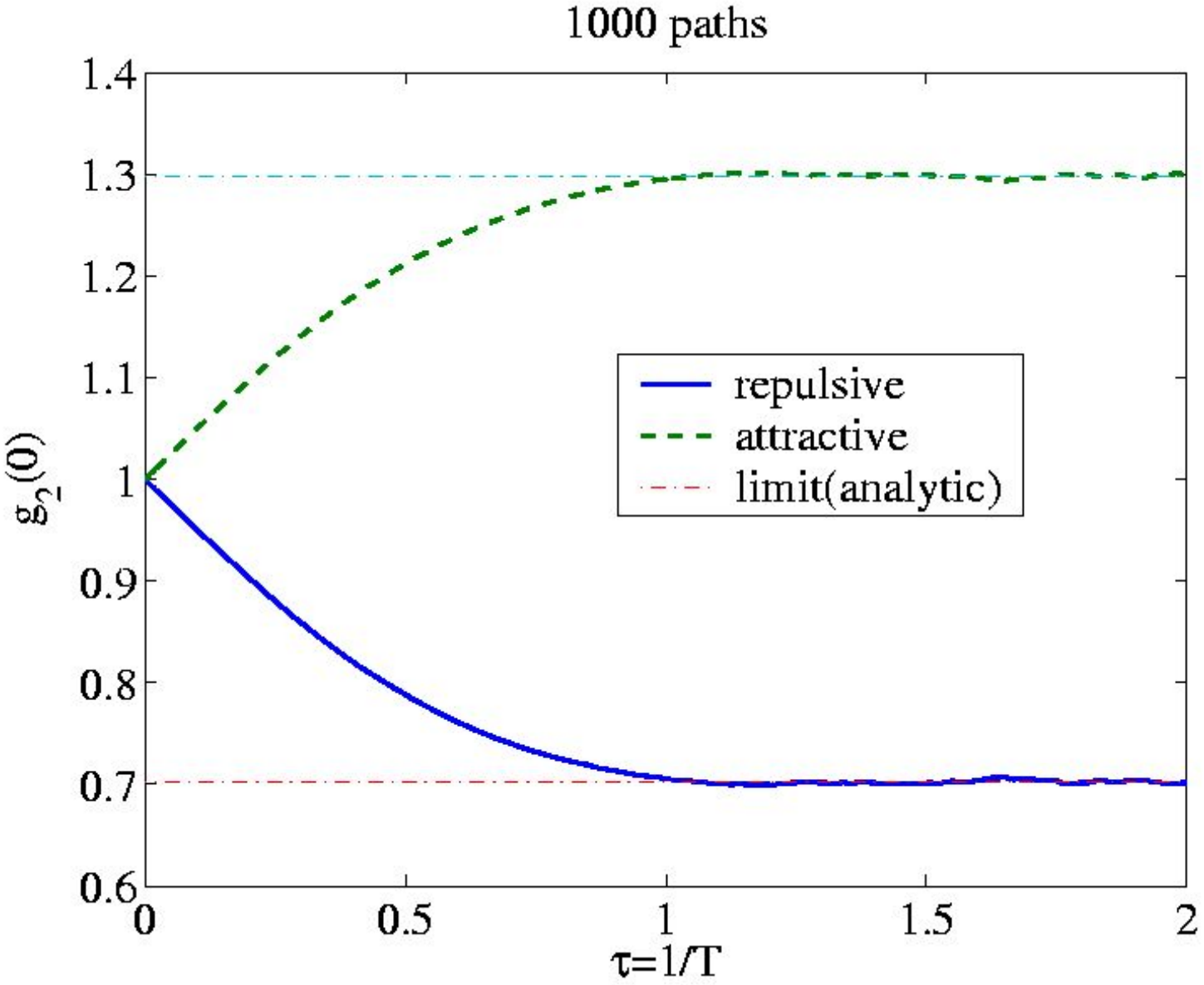
$$\frac{d\Omega}{d\tau} = -\Omega\left\{-t\sum_{\langle i,j\rangle,\sigma} n_{i,j.\sigma} + U\sum_{j} n_{j,j,\downarrow} n_{j,j,\uparrow} - \mu\sum_{j,\sigma} n_{j,j,\sigma}\right\}$$

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

where:

$$\Delta_{i,j,\sigma}^{(r)} = \left[-t\delta_{\langle i,j\rangle} + \delta_{i,j}\left\{U n_{j,j,\sigma'} - |U| n_{j,j,\sigma} + \frac{1}{2}|U| - \mu\right\}\right] \pm \delta\sqrt{2|U|}\,\xi_j^{(r)}$$

1D lattice – 100 sites



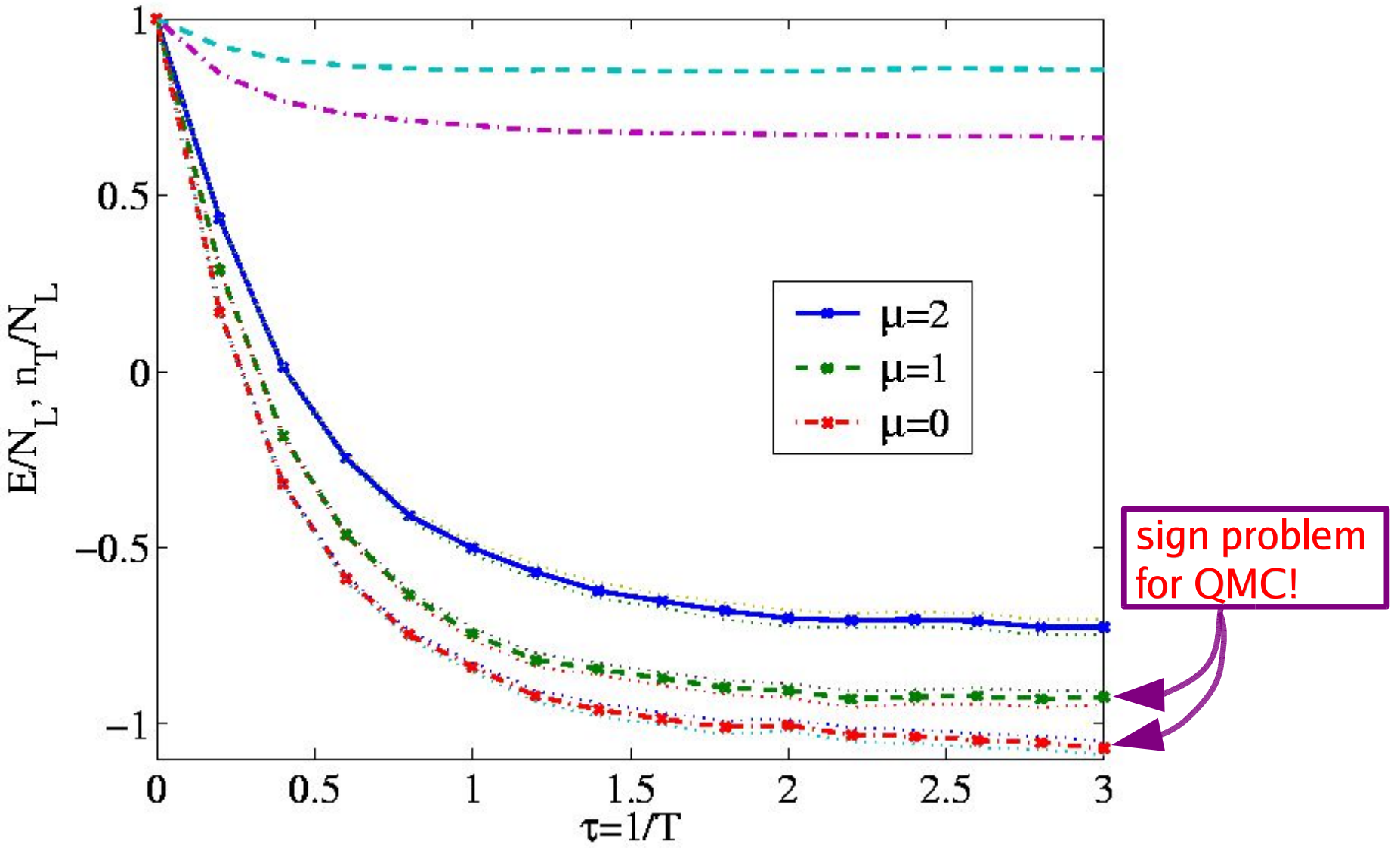
Branching

- averages are weighted, e.g.

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

- but weights spread exponentially
  - many irrelevant paths
  - so delete low-weight paths and clone high-weight paths
- branching algorithm increases sampling efficiency

2D – 16x16 sites



Summary: Hubbard simulations

- Gaussian operator basis for density operator
- first-principles, finite temperature calculations of Hubbard model
- 1, 2 and 3D simulations, up to 400 sites on a p.c.
- simple branching algorithm for weighted paths
- no evidence of a sign problem!

What's ahead for Gaussian methods?

- optimise for large lattices - memory, parallel machines
- optimise sampling - more sophisticated methods
- study continuous Fermi gas (BEC-BCS crossover)
- study atomic-molecular condensates
- explore first-principles dynamical (real-time) calculations

Conclusions

Ultracold gases are an elegant and well-controlled environment for exploring the fundamentals of quantum, many-body physics.

There is a need for simulation methods to study these systems from first principles.

Gaussian phase-space methods are well-placed to fill this need.

The fermionic Gaussian method successfully simulates the Hubbard model without sign error.

There are many more applications to come, for both fermions and bosons, both dynamical and equilibrium.