Gaussian quantum Monte-Carlo Methods

phase-space simulations of many-body systems

Joel Corney

corney@physics.uq.edu.au

ARC Centre of Excellence for Quantum-Atom Optics, The University of Queensland

Overview

- introduction to phase-space representations
  - $+P$ method
- Gaussian operator bases
  - overcompleteness and differential properties
- quantum evolution in real or imaginary time
  - mapping to stochastic phase-space equations
- application to Hubbard model
  - improvements through symmetry and gauge considerations

Overview

- **introduction to phase-space representations**
  - $+P$ method
- Gaussian operator bases
  - overcompleteness and differential properties
- quantum evolution in real or imaginary time
  - mapping to stochastic phase-space equations
- application to Hubbard model
  - improvements through symmetry and gauge considerations

Wigner distribution

- A classical state can be represented by a joint probability distribution in phase space $P(\mathbf{x},\mathbf{p})$
- 1932: Wigner[1] constructed analogous quantity for quantum states:

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

✔ Wigner function gives correct marginals:
$$\int dxW(x,p)=2\hbar P(p)$$
$$\int dpW(x,p)=2\hbar P(x)$$

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

1. E. P. Wigner, Phys. Rev. **40**, 749 (1932).

P and Q distrubutions

- other phase-space distributions were also defined by
  - Husimi[1]:

$$Q(\alpha) = \frac{1}{\pi}\left|\langle\Psi|\alpha\rangle\right|^2$$

  and

  - Glauber[2] and Sudarshan[3]:

$$|\Psi\rangle\langle\Psi| = \int d^2\alpha P(\alpha)|\alpha\rangle\langle\alpha|$$

1. K. Husimi, Proc. Phys. Math. Soc. Jpn. **22**, 264 (1940).
2. R. J. Glauber, Phys. Rev. **131**, 2766 (1963).
3. E. C. G. Sudarshan, Phys. Rev. Lett. **10**, 277 (1963).

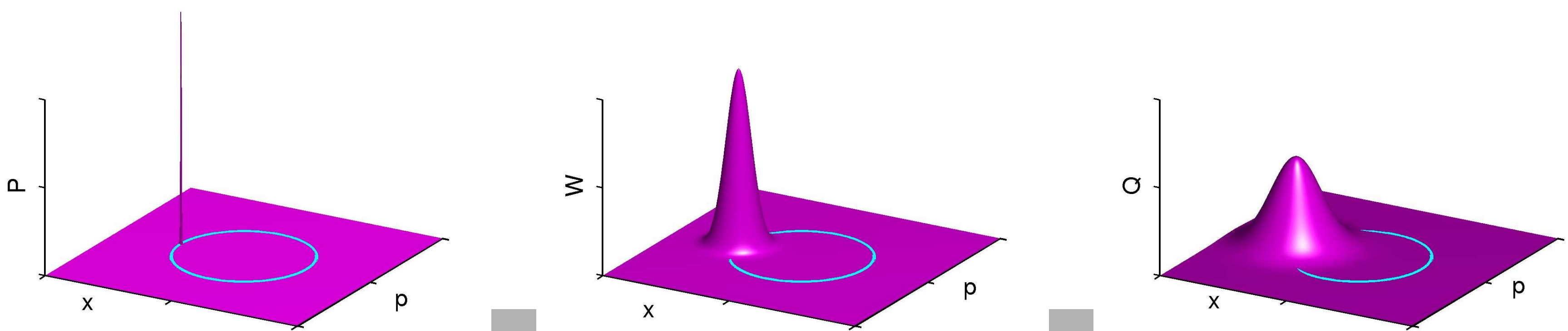
Phase-space distributions

- Wigner, Q and P all defined in terms of coherent states

$$\widehat{a}|\alpha\rangle = \alpha|\alpha\rangle; \;\; |\alpha\rangle \equiv \widehat{D}(\alpha)|0\rangle \equiv \exp[\alpha\widehat{a}^\dagger - \alpha^*\widehat{a}]|0\rangle$$

  - the distributions are interrelated by Gaussian convolutions
  - correspond to different choices of orderings:

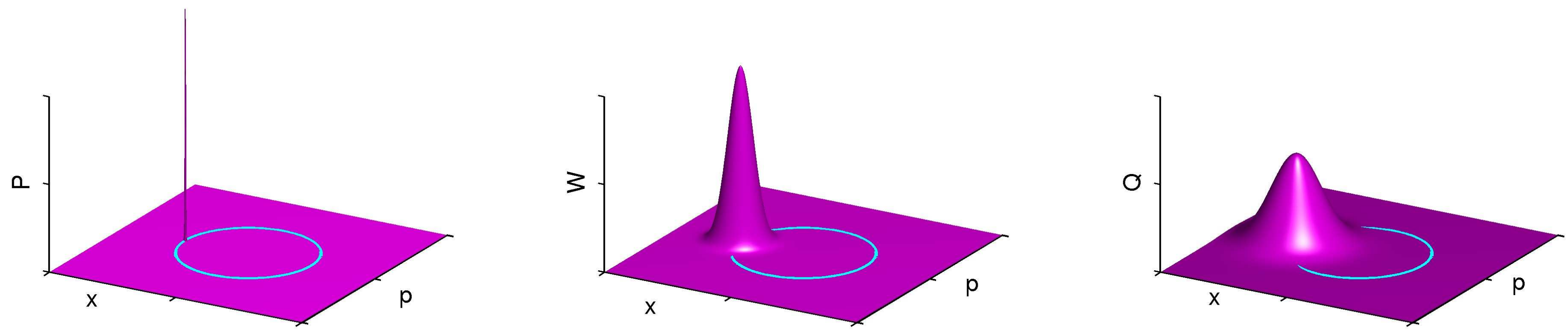
$$\langle\widehat{a}^\dagger\widehat{a}\rangle = \int d^2\alpha\left(|\alpha|^2 + n\right)p(\alpha); \;\; n = \begin{cases} 0 & p = P \\ -\frac{1}{2} & p = W \\ -1 & p = Q \end{cases}$$



Probability distributions

- to be a probabilistic representation, these 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 ✔

positive-P representation

- generalisation of the Glauber P by Drummond et al[1,2]
- expand $\widehat{\rho}$ over off-diagonal coherent-state projectors:

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

- off-diagonal coherent projectors are a very overcomplete basis
  - many equivalent $P(\alpha,\beta)$ functions for a given quantum state
  - can always find a positive one
  - time evolution of $\widehat{\rho}$ maps to diffusive evolution of $P(\alpha,\beta)$

1. S. Chaturvedi, P. D. Drummond, and D. F. Walls, J. Phys. A **10**, L187-192 (1977)
2. P. D. Drummond and C. W. Gardiner, J. Phys. A **13**, 2353 (1980).

positive-P Simulations

- maps state evolution onto two independent stochastic amplitudes:

$$\widehat{a} \rightarrow \alpha \quad \widehat{a}^{\dagger} \rightarrow \beta^{*}$$

- stochastic averages correspond to normally ordered correlations

$$\langle : f(\widehat{a}^{\dagger}, \widehat{a}) : \rangle = \int d^2\alpha \, d^2\alpha^{+} \, f(\beta^{*}, \alpha) P(\alpha, \beta)$$

- many applications in quantum optics and ultracold atoms
- both real time (dynamics) and imaginary time (finite temperature) calculations

positive-P Applications

- quantum optics
  - superfluorescence:
    - F. Haake et al, Phys. Rev. Lett. **42**, 1740 (1979)
    - P. D. Drummond and J. H. Eberly, Phys. Rev. A **25**, 3446 (1982).
  - parametric amplifiers:
    - C. W. Gardiner, *Quantum Noise,* (Springer-Verlag, Berlin, 1991).
  - quantum solitons:
    - S. J. Carter et al, Phys. Rev. Lett. **58**, 1841 (1987)
    - P. D. Drummond, R. M. Shelby, S. R. Friberg and Y. Yamamoto, Nature **365**, 307 (1993)
- ultracold gases
  - dynamics of Bose-Einstein condensates:
    - M. J. Steel, M. K. Olsen, L. I. Plimak *et al*, Phys. Rev. **A58**, 4824 (1998)
    - P. D. Drummond, J. F. Corney, Phys. Rev. **A 60**, R2661-R2664 (1999)
    - K. V. Kheruntsyan, M. K. Olsen, and P. D. Drummond, Phys. Rev. Lett. **95**, 150405 (2005).
  - finite-temperature correlations in Bose gases:
    - P. D. Drummond, P. Deuar and K. V. Kheruntsyan, Phys. Rev. Lett. **92**, 040405 (2004).

Example: Evaporative Cooling of a BEC

$$\widehat{H} = \int d^3\mathbf{x}\widehat{\Psi}^\dagger(\mathbf{x},t)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x},t) + \frac{U}{2}\widehat{\Psi}^\dagger(\mathbf{x},t)\widehat{\Psi}(\mathbf{x},t)\right]\widehat{\Psi}(\mathbf{x},t)$$

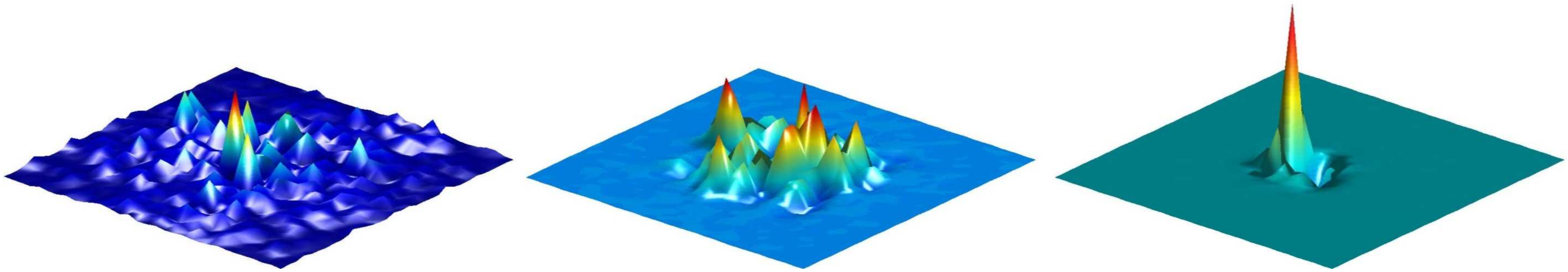
- equivalent (Itô) stochastic equations($j = 1,2$):

$$i\hbar\frac{\partial\psi_j}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + 4\pi a_0\frac{\hbar^2}{m}\psi_j\psi^*_{3-j} + V(\mathbf{x},t) + \xi_j(\mathbf{x},t)\right]\psi_j$$

- quantum noise:

$$\langle\xi_{j'}(\mathbf{x}',t')\xi_j(\mathbf{x},t)\rangle = i\frac{4\pi a_0\hbar^3}{m}\delta_{jj'}\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

Example: Evaporative Cooling of a BEC



- 3D calulation with 20000 atoms, 32000 modes
- start with Bose gas above T_c; finish with narrow BEC peak

✘ Problems!

  - ✘ method pushed to the limit
  - ✘ breaks down for longer times, stronger interactions

What about fermions?

- $+P$ is defined only for bosonic systems
- could we use fermionic coherent states[1,2]? $\widehat{c}|\gamma\rangle = \gamma|\gamma\rangle$
  - like bosonic counterparts, have useful completeness properties
  - require anticommuting, Grassmann variables: $\gamma_1\gamma_2 = -\gamma_2\gamma_1$
- Cahill and Glauber constructed fermionic representations[3]
- numerical simulations implemented[4], but do not scale well
- the Grassmann algebra introduces great computational complexity

1. J. L. Martin, Proc. Roy. Soc. **A 251**, 543 (1959)
2. Y. Ohnuki and T. Kashiwa, Prog. Theor. Phys. **60**, 548 (1978).
3. K. E. Cahill and R. J. Glauber, Phys. Rev. **A 59**, 1538 (1999)
4. L. I. Plimak, M. J. Collett and M. K. Olsen, Phys. Rev. A **64**, 063409 (2001)

Phase-space representation

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

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

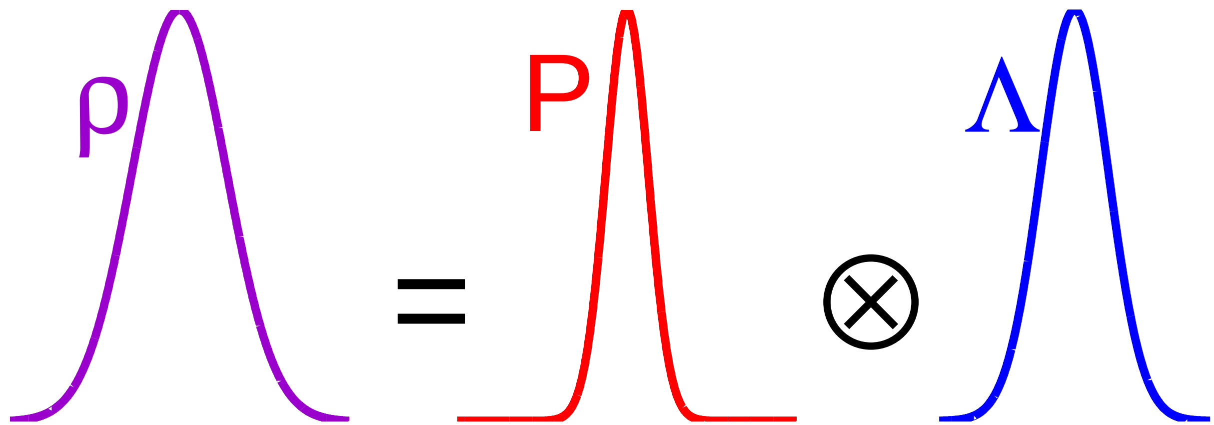
$$\hat{\rho} = E\left[\hat{\Lambda}(\overrightarrow{\lambda})\right]$$

Overview

- introduction to phase-space representations
  - $+P$ method
- **Gaussian operator bases**
  - overcompleteness and differential properties
- quantum evolution in real or imaginary time
  - mapping to stochastic phase-space equations
- application to Hubbard model
  - improvements through symmetry and gauge considerations

Operator Bases

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



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

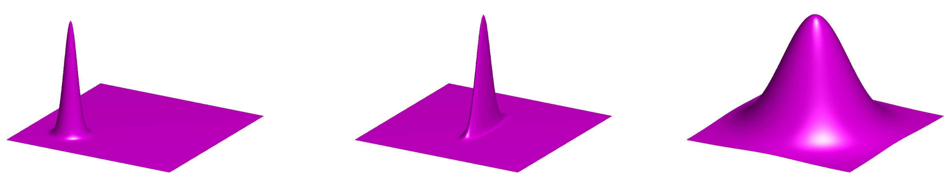
Required Properties

- to enable a phase-space representation, the operators $\widehat{\Lambda}(\overrightarrow{\lambda})$ must
  1. form a *complete* basis for the class of physical density matrices
  2. possess a *second-order differential* form for all two-body operators
  3. represent any state by a *positive* expansion
  4. be *analytic* functions of the phase-space variables
- 3 and 4 are obtained with *non-Hermitian* elements in the basis
- 2 and 4 $\Longrightarrow$ quantum evolution maps to a Fokker-Planck equation for a diffusive process

General Gaussian operators

generalisation of density operators that describe Gaussian states

- Gaussian states can be:
  - coherent (for bosons), squeezed (eg BCS), 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: General form

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

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

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

- Ω: weight (for gauges and unnormalised density matrices)
- α and α^{+}: coherent amplitudes
- $\mathbf{n}$: complex number correlations (normal fluctuations)
- $\mathbf{m}$ and $\mathbf{m}^{+}$: independent squeezing (anomalous) correlations

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

$\Longrightarrow$ phase-space dimension: $\leq \begin{cases} 2(1-M+2M^{2}) & \text{for fermions} \\ 2(1+3M+2M^{2}) & \text{for bosons} \end{cases}$

Moments

- observables are weighted averages ($E[A] \equiv \int d\lambda \Omega A P(\lambda) / \int d\lambda \Omega P(\lambda)$):

$$
\begin{aligned}
\langle \widehat{a}_i \rangle &= E[\alpha_i] \\
\left\langle \widehat{a}_i^\dagger \widehat{a}_j \right\rangle &= E\left[\alpha_i^+ \alpha_j + n_{ij}\right] \\
\left\langle \widehat{a}_i \widehat{a}_j \right\rangle &= E\left[\alpha_i \alpha_j + m_{ij}\right]
\end{aligned}
$$

- higher-order moments (normally ordered) are averages of Wick decompositions, eg:

$$
\langle : \widehat{n}_i \widehat{n}_j : \rangle = E\left[n_{ii} n_{jj} - n_{ij} n_{ji} + m_{ij}^+ m_{ji}\right]
$$

Non-Hermitian Elements

- when $\alpha^* = \alpha^+$, $\mathbf{m}^\dagger = \mathbf{m}^+$, and $\mathbf{n}^\dagger = \mathbf{n}$, the Gaussian operators correspond to density operators for physical states
- full Gaussian basis also includes non-Hermitian generalisations of these operators

  $\Longrightarrow$ gives the overcompleteness necessary to ensure properties
  - 3: positivity, and
  - 4: freedom to diffuse

- for more on the properties of generalised Gaussian operators, see: J. F. Corney and P. D. Drummond, J. Phys. A **39**, 269 (2006).
- the Hubbard-Stratonovich transformation, as used in Auxiliary field methods, gives exponentials of one-body operators (and thus Gaussian operators), but the approach is somewhat different. See e.g. S. Roumbouts and K. Heyde, Phys. Status. Solidi B **237**, 99 (2003).

Differential Identities

- all one-body operators equate to first-order derivatives:

$$
\begin{aligned}
\widehat{\Lambda} &= \underline{\Omega}\frac{\partial\Lambda}{\partial\underline{\Omega}} \\
:\widehat{\underline{a}}\widehat{\Lambda}: &= \underline{\alpha}+\underline{\underline{\sigma}}\frac{\partial\widehat{\Lambda}}{\partial\underline{\alpha}^{+}} \\
:\delta\widehat{\underline{a}}\delta\widehat{\underline{a}}^{\dagger}\widehat{\Lambda}: &= \underline{\underline{\sigma}}\widehat{\Lambda}\pm\underline{\underline{\sigma}}\frac{\partial\widehat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}} \\
\left\{\delta\widehat{\underline{a}}:\delta\widehat{\underline{a}}^{\dagger}\widehat{\Lambda}:\right\} &= \pm\underline{\underline{\sigma}}\widehat{\Lambda}+\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\frac{\partial\widehat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}} \\
\left\{\delta\widehat{\underline{a}}\delta\widehat{\underline{a}}^{\dagger}\widehat{\Lambda}\right\} &= \left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\widehat{\Lambda}\pm\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\frac{\partial\widehat{\Lambda}}{\partial\underline{\underline{\sigma}}}\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)
\end{aligned}
$$

Special case I: Coherent-state projectors

- for bosons, we can restrict the basis to $\vec{\lambda} = (\Omega, \alpha, (\alpha^+)^*, \mathbf{0}, \mathbf{0}, \mathbf{0})$:
- get the kernal for the $+P$ representation

$$\widehat{\Lambda} \;=\; \Omega \frac{|\alpha\rangle\langle(\alpha^+)^*|}{\langle(\alpha^+)^*|\alpha\rangle}$$

- differential identities reduce to

$$\widehat{\mathbf{a}}\widehat{\Lambda} = \alpha\widehat{\Lambda}; \qquad \widehat{\mathbf{a}}^\dagger\widehat{\Lambda} = \left(\alpha^+ + \frac{\partial}{\partial\alpha}\right)\widehat{\Lambda}$$

$$\widehat{\Lambda}\widehat{\mathbf{a}} = \left(\alpha + \frac{\partial}{\partial\alpha^+}\right)\widehat{\Lambda}; \qquad \widehat{\Lambda}\widehat{\mathbf{a}}^\dagger = \alpha^+\widehat{\Lambda}$$

Special case II: Thermal operators

- for a number-conserving system, can restrict basis to $\overrightarrow{\lambda} = (\Omega, \mathbf{0}, \mathbf{0}, \mathbf{n}, \mathbf{0}, \mathbf{0})$:

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

- defined for bosons (upper sign) and *fermions* (lower sign)
- moments:

$$\left\langle \widehat{a}_i \widehat{a}_j \right\rangle = 0; \qquad \left\langle \widehat{a}_i^{\dagger} \widehat{a}_j \right\rangle = E\left[n_{ij}\right]$$

$$\left\langle \widehat{a}_i^{\dagger} \widehat{a}_j^{\dagger} \widehat{a}_j \widehat{a}_i \right\rangle = E\left[n_{ii} n_{jj} \pm n_{ij} n_{ji}\right]$$

Special case II: Thermal operator identities

$$
\begin{aligned}
\widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^{T}\widehat{\Lambda} &= \mathbf{n}\widehat{\Lambda} + (\mathbf{I}-\mathbf{n})\frac{\partial\widehat{\Lambda}}{\partial\mathbf{n}}\mathbf{n}\,, \\
\widehat{\Lambda}\widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^{T} &= \mathbf{n}\widehat{\Lambda} + \mathbf{n}\frac{\partial\widehat{\Lambda}}{\partial\mathbf{n}}(\mathbf{I}-\mathbf{n})\,, \\
\widehat{\mathbf{b}}^{\dagger T}\widehat{\Lambda}\widehat{\mathbf{b}}^{T} &= (\mathbf{I}-\mathbf{n})\widehat{\Lambda} + (\mathbf{I}-\mathbf{n})\frac{\partial\widehat{\Lambda}}{\partial\mathbf{n}}(\mathbf{I}-\mathbf{n})\,, \\
\left(\widehat{\mathbf{b}}\widehat{\Lambda}\widehat{\mathbf{b}}^{\dagger}\right)^{T} &= \mathbf{n}\widehat{\Lambda} - \mathbf{n}\frac{\partial\widehat{\Lambda}}{\partial\mathbf{n}}\mathbf{n}
\end{aligned}
$$

- where $\tilde{\mathbf{n}} = \mathbf{I} \pm \mathbf{n}$ is the hole correlations
- for two-body operators, apply two of these identities in succession

Overview

- introduction to phase-space representations
  - $+P$ method
- Gaussian operator bases
  - overcompleteness and differential properties
- **quantum evolution in real or imaginary time**
  - mapping to stochastic phase-space equations
- application to Hubbard model
  - improvements through symmetry and gauge considerations

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

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

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

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**: the operators to differential form: $\widehat{L}\left[\widehat{\Lambda}\right] = \mathcal{L}\widehat{\Lambda}$
4. **Integrate** by parts: $\int P\mathcal{L}\widehat{\Lambda} d\overrightarrow{\lambda} \Longrightarrow \int \widehat{\Lambda}\mathcal{L}' P d\overrightarrow{\lambda}$
   - neglect boundary terms (for sufficiently bounded P)
     - $\Longrightarrow$ analyse stability of resulting phase-space trajectories
     - $\Longrightarrow$ monitor tails of P during simulation
5. **Obtain** Fokker-Planck equation: $\partial P/\partial\tau = \mathcal{L}' P$

Fokker-Planck equations

- resulting Fokker-Planck equation is of the form

$$\frac{d}{dt}P(\overrightarrow{\lambda},\tau) = \left[-\sum_{a=0}^{p}\frac{\partial}{\partial\lambda_a}A_a(\overrightarrow{\lambda})+\frac{1}{2}\sum_{a,b=0}^{p}\frac{\partial}{\partial\lambda_a}\frac{\partial}{\partial\lambda_b}D_{ab}(\overrightarrow{\lambda})\right]P(\overrightarrow{\lambda},\tau)$$

  - A_a gives the drift (deterministic component)
  - D_{ab} gives the diffusion (stochastic component)
- D_{ab} must be positive-definite (in terms of real variables)
  - always possible by appropriate choice of derivatives:

$$\partial/\partial\lambda_a = \partial/\partial\lambda_a^x = -i\partial/\partial\lambda_a^y$$

  - freedom in derivatives comes from analyticity (overcompleteness)

Itô stochastic equations

- sample with Itô stochastic equations for $\overrightarrow{\lambda}$

$$d\lambda_a(\tau) \quad = \quad A_a(\overrightarrow{\lambda})\,d\tau + \sum_b B_{ab}(\overrightarrow{\lambda})\,dW_b(\tau)$$

  - where $dW_b(\tau)$ are Weiner increments, obeying

$$\left\langle dW_b(\tau)\,dW_{b'}(\tau')\right\rangle = \delta_{b,b'}\delta(\tau-\tau')d\tau$$

    - i. e. Gaussian white noise
  - noise matrix B_{ab} is obtained by

$$D_{ab} = \sum_c B_{ac}B_{bc}$$

Stratonovich stochastic equations

- multiplicative SDEs do not obey the normal rules of calculus

  $\Longrightarrow$ must take care to choose the appropriate numerical algorithm
- solution to Itô equations is obtained by an explicit (Euler) algorithm
- for solution by a semi-implicit method, must start from equivalent Stratonovich equations:

$$d\lambda_a = \left[A_a(\overrightarrow{\lambda}) - \frac{1}{2}\sum_{bc} B_{cb}(\overrightarrow{\lambda}) \frac{\partial B_{ab}(\overrightarrow{\lambda})}{\partial \lambda_c} \right] d\tau + \sum_b B_{ab}(\overrightarrow{\lambda})\, dW_b$$

  - i.e. the drift is modified

Stochastic Gauges

- mapping from Hilbert space to phase space not unique

  $\Longrightarrow$ many “gauge” choices

- can alter noise terms B_{ij} (diffusion gauge[1])
- can introduce arbitrary drift functions $g_j(\overrightarrow{\lambda})$ (drift gauge[2])

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

Trajectory $$d\lambda_i = A_i \, d\tau + B_{ij} [dW_j - g_j \, d\tau]$$

- can also choose different bases, identities

1. L. I. Plimak, M. K. Olsen and M. J. Collett, Phys. Rev. A **64**, 025801 (2001)
2. P. Deuar and P. D. Drummond, Comp. Phys. Commun. **142**, 442 (2001); Phys. Rev. A **66**, 033812 (2002); J. Phys. A: Math. Gen. 39, 2723 (2006)

Interacting many-body physics

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

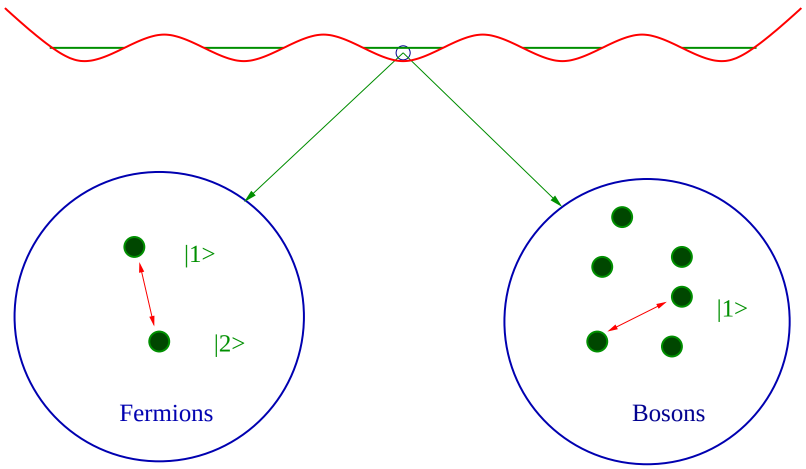
- ✔ many-body problems map to nonlinear stochastic equations
- ✔ calculations can be from first principles
- ✔ precision limited only by sampling error
- ✔ choose basis to suit the problem

- for more details on the Gaussian method for fermions, see J. F. Corney and P. D. Drummond, Phys. Rev. B **73** 125112 (2006).

Overview

- introduction to phase-space representations
  - $+P$ method
- Gaussian operator bases
  - overcompleteness and differential properties
- quantum evolution in real or imaginary time
  - mapping to stochastic phase-space equations
- **application to Hubbard model**
  - improvements through symmetry and gauge considerations

Application: Hubbard model



$$\widehat{H} = -\sum_{ij,\sigma} t_{ij} \widehat{c}^{\dagger}_{i,\sigma} \widehat{c}_{j,\sigma} + U \sum_{j} \widehat{c}^{\dagger}_{j,\uparrow} \widehat{c}^{\dagger}_{j,\downarrow} \widehat{c}_{j,\downarrow} \widehat{c}_{j,\uparrow}$$

- 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

Applying the Gaussian representation

- Use thermal basis, and apply mappings

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

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

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

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

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

Positive-Definite Diffusion

- Modify interaction term with a ‘Fermi gauge’:

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

$\Longrightarrow$ 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

$\Longrightarrow$ weights Ω guaranteed to be *positive*

Itô Equations

- Itô stochastic equations, in matrix form:

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

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

where the stochastic propagator matrix is

$$T_{ij,\sigma}^{(r)} = -t_{ij} + \delta_{ij}\left\{Un_{jj,\sigma'} - \mu \pm \sqrt{2|U|}\xi_j^{(r)}\right\}$$

- $\xi_j^{(r)}$ are delta-correlated white noises:

$$\langle \xi_j^{(r)}(\tau)\,\xi_{j'}^{(r')}(\tau')\rangle = \delta_{j,j'}\delta_{r,r'}\delta(\tau-\tau')$$

Stratonovich Equations

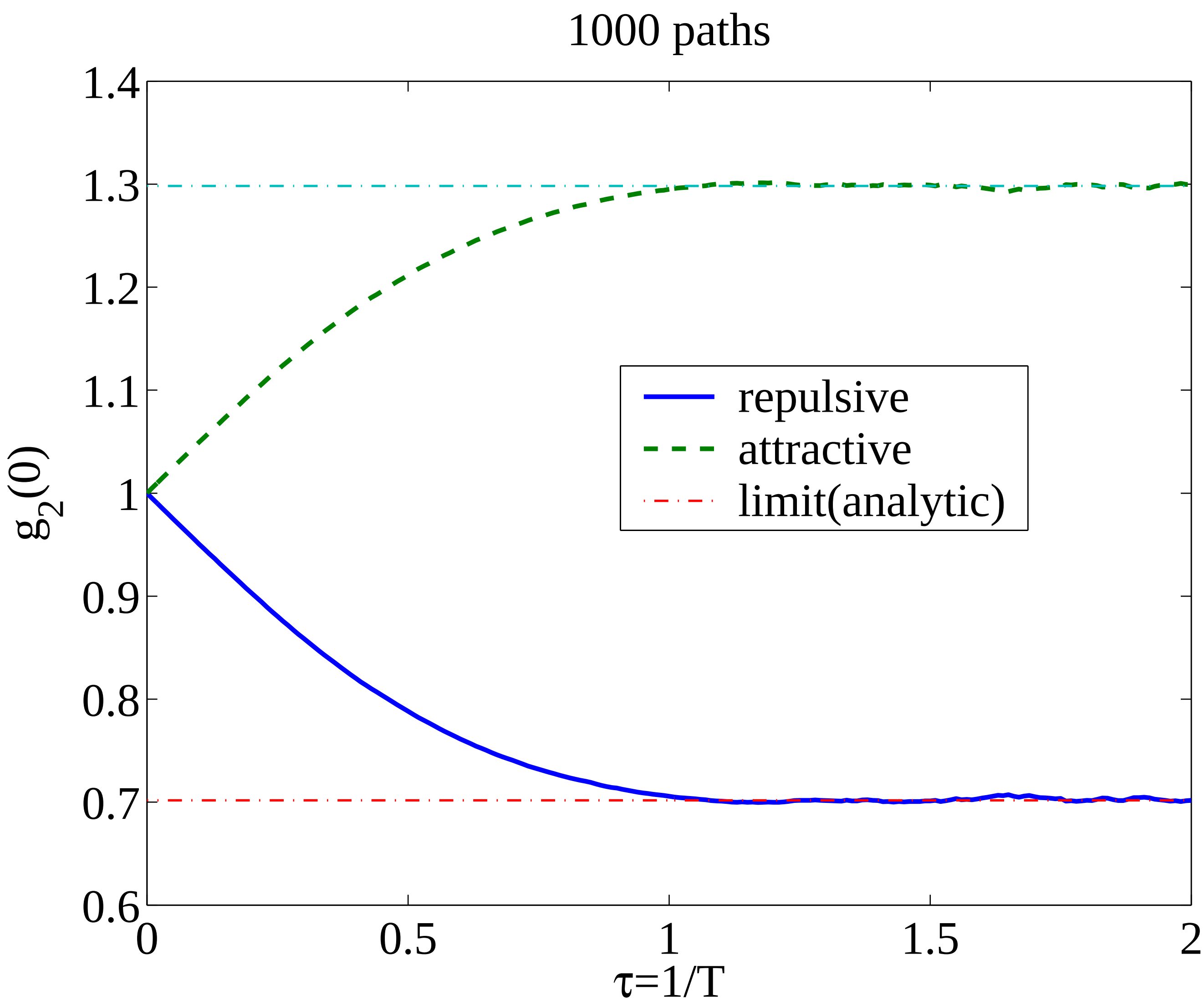
- in Stratonovich form, the stochastic propagator matrix is

$$T_{ij,\sigma}^{(r)} = -t_{ij} + \delta_{ij}\left\{U\left(n_{jj,\sigma'} - n_{jj,\sigma} + \frac{1}{2}\right) - \mu \pm \sqrt{2|U|}\xi_j^{(r)}\right\}$$

- we use an iterative, semi-implicit algorithm[1], with an adaptive step-size to overcome stiffness
- for more on the Hubbard calculation, see 2 and 3

1. P.D. Drummond and I.K. Mortimer, J. Comp. Phys. 93 (1991) 144.
2. J. F. Corney and P. D. Drummond, Phys. Rev. Lett. **93**, 260401 (2004)
3. P. D. Drummond and J. F. Corney, Comput. Phys. Commun. **169**, 412 (2005)

1D Lattice-100 sites



Branching

- averages are weighted,eg

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

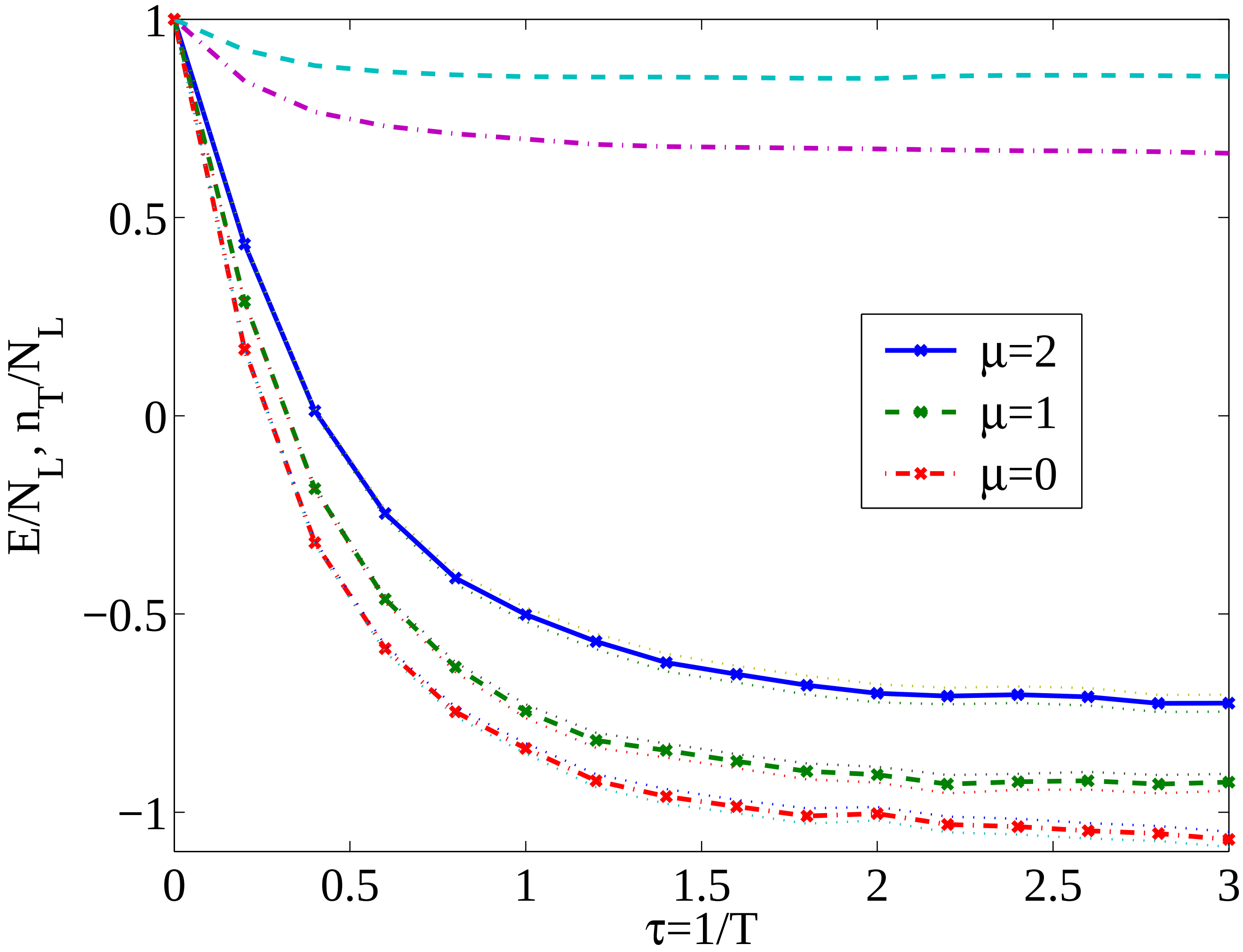
✘ but weights spread exponentially $\Longrightarrow$ many irrelevant paths

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

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

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

16x16 2D Lattice



Symmetry Projection Schemes

- 4×4 , 16×16 calculations showed that sampling error was well controlled for various filling factors - including those for which other methods suffer a severe sign problem
- more precise simulations at Würzburg and Zürich showed inaccuracies at large β for some correlation functions
- but true ground-state results could be obtained by supplementing with a symmetry projection scheme[1]
    - trade-off is an increase in sampling error

1. F. F. Assaad, P. Werner, P. Corboz, E. Gull and M. Troyer, Phys. Rev. B **72**, 224518 (2005)

Symmetry Preservation

- *problem*: chosen basis does not reflect all symmetries of the Hamiltonian
  - in principle, distribution will restore the symmetry
  - but broad tails mean that
    - accurate sampling is difficult
    - possibility of boundary-term errors
- *possible solution*:
  - use basis that possesses Hamiltonian symmetries
  - use stochastic gauges to ensure boundedness of P

Summary

- Generalised phase-space representations provide a means of simulating many-body quantum physics from first principles
- Coherent-state-based methods have been successful in simulating quantum dynamics of photons and weakly interacting bosons.
- Gaussian-based methods extend the applicability to highly correlated systems of bosons and *fermions*.
- Simulated the Hubbard model, apparently *without sign errors*.
- Some inaccuracies at low temperature can be overcome by:
  - supplementary *symmetry projection*, or
  - possibly by *basis* and *stochastic gauge* choice.