Fermionic phase-space method for exact quantum dynamics

Magnus Ögren

School of Science and Technology,
Örebro University, Sweden.
&
Nano-Science Center,
University of Copenhagen, Denmark.

Thanks to: Joel Corney, Karén Kheruntsyan and Claudio Verdozzi

Outline of the presentation:

Specific examples from the use of the Gaussian phase-space method for fermions. Mainly from the modeling of dissociation of molecular Bose-Einstein condensates (MBEC) into pair-correlated fermionic atoms, also the Hubbard model:

I Briefly explain the underlying physical problem, report on numerical results, and the comparison with other methods of quantum dynamics.

II How can we improve the performance, and benchmark the accuracy of the method for such large system such that we cannot compare with independent methods.

What is the problem I ?

Fermi-Bose model (e.g. molecule --> atoms reaction)

$$\hat{H} = \hat{H}_0 - i\hbar\chi \int d\mathbf{x} \left(\hat{\Psi}_0^\dagger \hat{\Psi}_2 \hat{\Psi}_1 - \hat{\Psi}_1^\dagger \hat{\Psi}_2^\dagger \hat{\Psi}_0 \right)$$

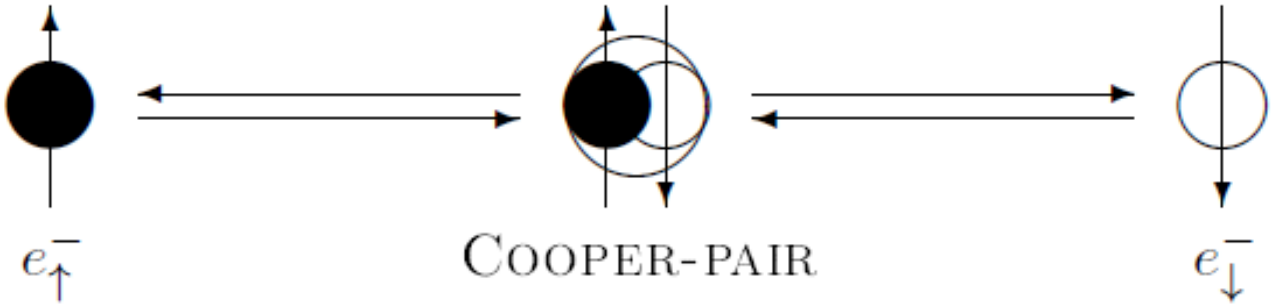
Fermi-Bose model (simplified to a uniform molecular field)

$$\widehat{H} = \hbar \sum\nolimits_{\mathbf{k},\sigma} \Delta_{\mathbf{k}} \hat{n}_{\mathbf{k},\sigma} - i\hbar\kappa \sum\nolimits_{\mathbf{k}} \left(\hat{a}^\dagger \hat{m}_{\mathbf{k}} - \hat{m}_{\mathbf{k}}^\dagger \hat{a} \right)$$

$$\hat{n}_{\mathbf{k},\sigma} = \hat{c}_{\mathbf{k},\sigma}^\dagger \hat{c}_{\mathbf{k},\sigma} \quad \text{and} \quad \hat{m}_{\mathbf{k}} = \hat{c}_{\mathbf{k},1} \hat{c}_{-\mathbf{k},2} \qquad \hbar\Delta_{\mathbf{k}} \equiv \hbar^2 |\mathbf{k}|^2 / (2m_a) + \hbar\Delta$$

Application 1: Superconductivity

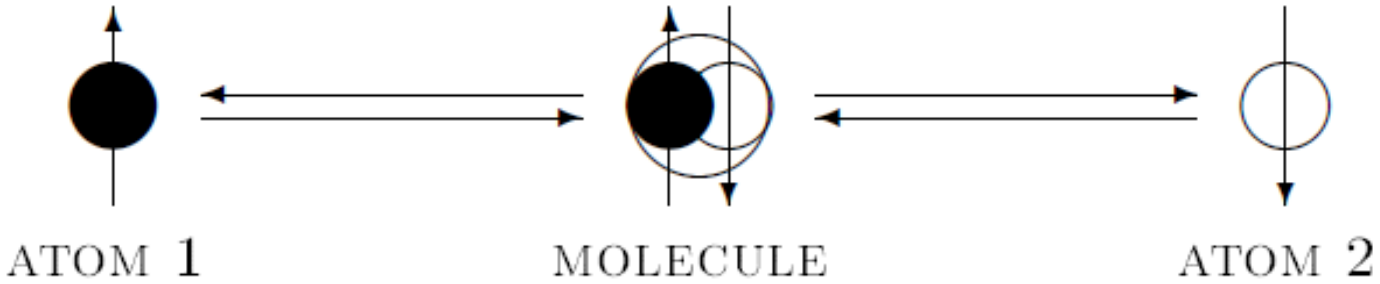
Friedberg R and Lee T D 1989 *Phys. Rev.* B **40** 6745



Nuclear physics?

Application 2: Dissociation of ultra-cold molecules

Poulsen U V and Mølmer K 2001 *Phys. Rev.* A **63** 023604



Does the simplest mean-field description work here?

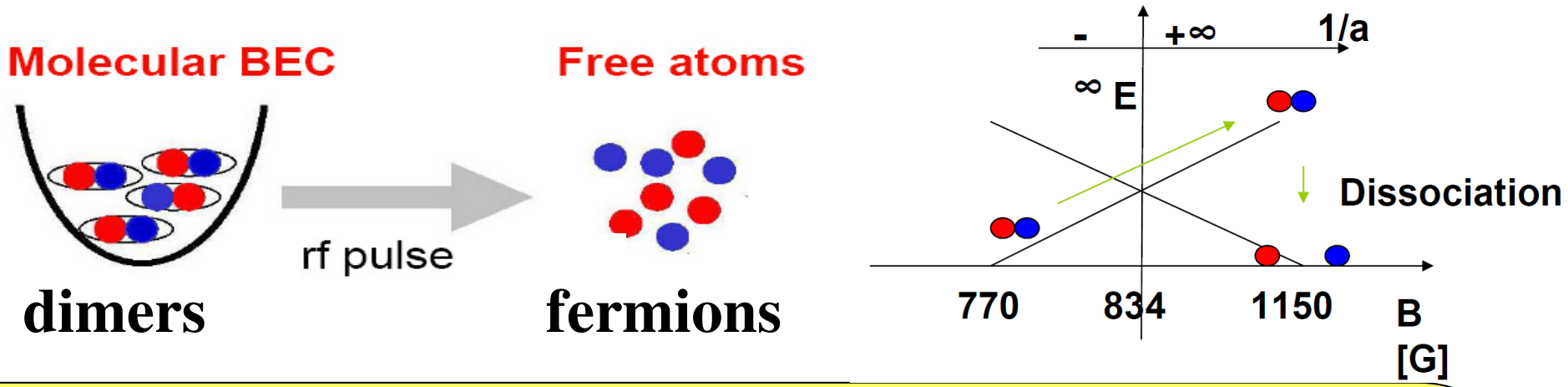
* Gross-Pitaevskii type equations for molecular dissociation into bosonic atoms:

, the corresponding set of coupled equations for the molecular and atomic mean-fields, Ψ_0 and Ψ_1, respectively, can be written as

$$\begin{aligned} \frac{\partial \Psi_0}{\partial t} &= i\frac{\hbar}{2m_0}\frac{\partial^2 \Psi_0}{\partial x^2} - \frac{\chi}{2}\Psi_1^2, \\ \frac{\partial \Psi_1}{\partial t} &= i\left[\frac{\hbar}{2m_1}\frac{\partial^2}{\partial x^2} - \Delta\right]\Psi_1 + \chi\Psi_0\Psi_1^*. \end{aligned} \tag{2.11}$$

With initially no atoms present we have $\Psi_1(0) = 0$, and all the terms in the right-hand-side of the second equation will remain zero at all times, $N_1(t) = \int dx \Psi_1^* \Psi_1 = 0$, such that no increase in the atom number is possible. In contrast to this, theoretical approaches that do take into account quantum fluctuations (see Section 2.5.2), do predict the build-up of atomic population via a spontaneous emission process, and we therefore conclude that the

Motivation to study dissociation into fermions:



i) Conceptual:

Molecular dissociation as a fermionic analog of optical parametric down-conversion, a good candidate for developing the paradigm of *fermionic quantum atom optics*.

ii) Pragmatic:

Can we explain the experimentally observed atom-atom correlations.
(Molecules made up of fermions have longer lifetime.)
Development of computational tools for fermions.

Pairing mean-field theory (PMFT)

Here for a uniform system:

Well known Heisenberg's equations: **(e.g.** $\frac{d\hat{a}}{dt} = \frac{1}{i\hbar}\left[\hat{a}, \hat{H}\right]$ **)**

$$
\begin{cases}
\frac{d\hat{n}_{\mathbf{k},\uparrow}}{dt} = \kappa_D \left(\hat{a}\hat{m}_{\mathbf{k}}^{\dagger} + \hat{a}^{\dagger}\hat{m}_{\mathbf{k}}\right) \\
\frac{d\hat{n}_{\mathbf{k},\downarrow}}{dt} = \kappa_D \left(\hat{a}\hat{m}_{\mathbf{k}}^{\dagger} + \hat{a}^{\dagger}\hat{m}_{\mathbf{k}}\right) \\
\frac{d\hat{m}_{\mathbf{k}}}{dt} = -2i\Delta_{\mathbf{k}}\hat{m}_{\mathbf{k}} + \kappa_D \hat{a}\left(1 - \hat{n}_{\mathbf{k},\uparrow} - \hat{n}_{-\mathbf{k},\downarrow}\right) \\
\frac{d\hat{m}_{\mathbf{k}}^{\dagger}}{dt} = 2i\Delta_{\mathbf{k}}\hat{m}_{\mathbf{k}}^{\dagger} + \kappa_D \hat{a}^{\dagger}\left(1 - \hat{n}_{\mathbf{k},\uparrow} - \hat{n}_{-\mathbf{k},\downarrow}\right) \\
\frac{d\hat{a}}{dt} = -\kappa_D \sum_{\mathbf{k}} \hat{m}_{\mathbf{k}} \\
\frac{d\hat{a}^{\dagger}}{dt} = -\kappa_D \sum_{\mathbf{k}} \hat{m}_{\mathbf{k}}^{\dagger}
\end{cases}
\tag{10}
$$

This is a system of non-linear operator (ordinary) differential equation, that no physicist knows how to solve directly.

Factorization of expectation values gives c-number equations.

Pairing mean-field theory

the equations of motion in terms of the expectation values take the following form:

$$\begin{aligned}
\frac{dn_{\mathbf{k}}}{dt} &= \kappa\left(\beta^* m_{\mathbf{k}} + \beta m_{\mathbf{k}}^*\right), \\
\frac{dm_{\mathbf{k}}}{dt} &= -2i\Delta_{\mathbf{k}} m_{\mathbf{k}} + \kappa\beta\left(1 \pm 2n_{\mathbf{k}}\right), \\
\frac{d\beta}{dt} &= -\kappa \sum_{\mathbf{k}} m_{\mathbf{k}},
\end{aligned} \tag{2.19}$$

where $\kappa_D = \chi/L^D$, $\Delta_{\mathbf{k}} = \hbar\mathbf{k}^2/(2m) + \Delta$, and the $+$ $(-)$ sign refers to the case of bosonic (fermionic) atoms. From these equations we immediately see that in contrast to the Gross-Pitaevskii mean-field treatment, the pairing mean-field equations allow for the initiation of the population in the atomic fields (initially in the vacuum state) via the unity term in the

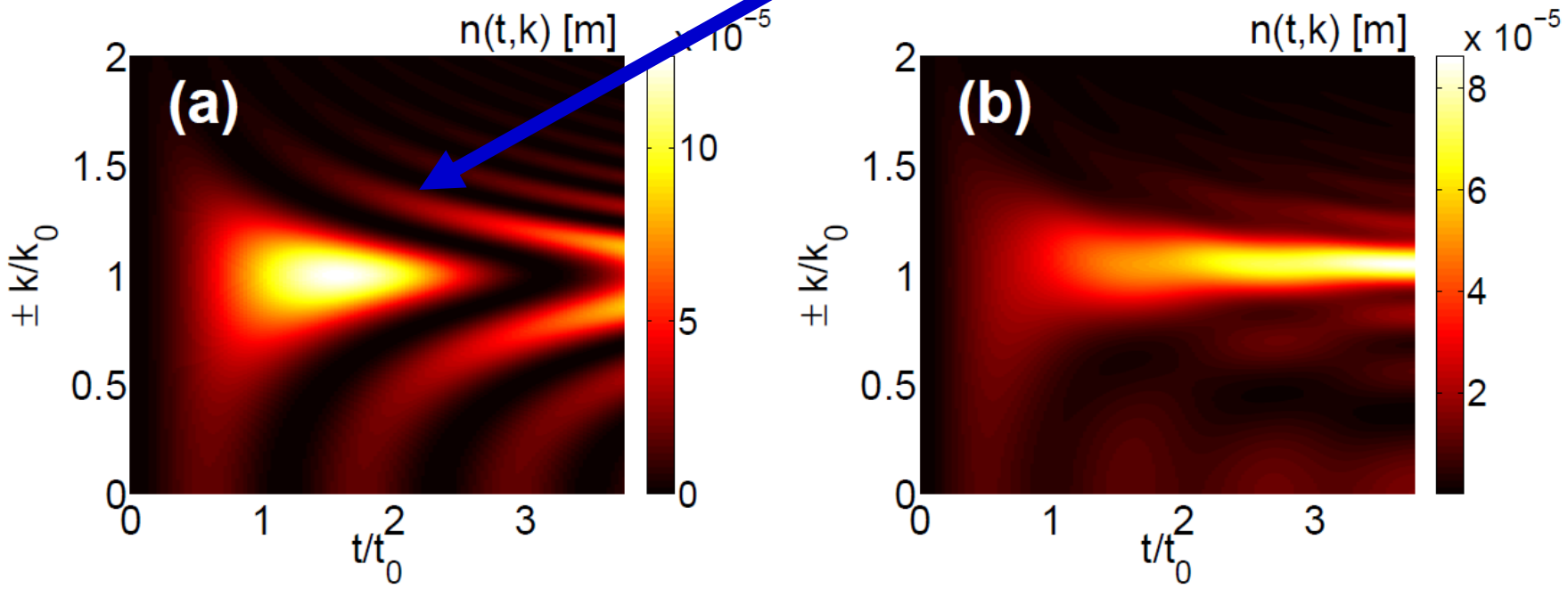
*** Note: Becomes linear if the molecules are undepleted (UMF).**

*** Note: The "1:s" are instrumental in initiating dissociation-dynamics, compare to 'GPE' mean-field equations.**

Pairing mean-field theory

Takes into account the depletion of the bosonic field.
This is needed when the number of molecules are small compared to the available atomic modes.
For a uniform field:

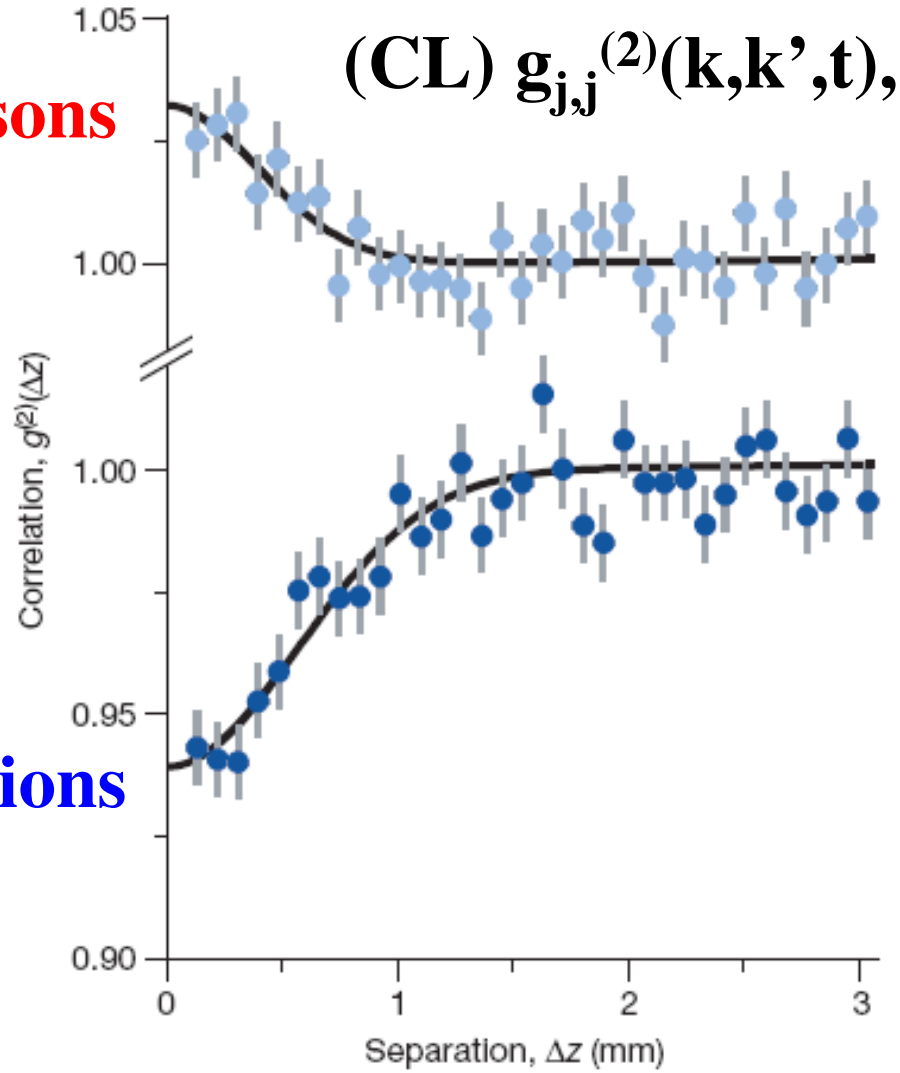
$$n_{\mathrm{k},\sigma}(t) \equiv \langle \hat{n}_{\mathrm{k},\sigma} \rangle = \left\langle \hat{a}^{\dagger}_{\mathrm{k},\sigma} \hat{a}_{\mathrm{k},\sigma} \right\rangle = \frac{g_0^2}{\Delta_{\mathrm{k}}^2 - q g_0^2} \sin^2\left(\sqrt{\Delta_{\mathrm{k}}^2 - q g_0^2}\, t \right)$$



Observations from the field of ultra-cold atoms:

Bosons

(CL) $g_{j,j}^{(2)}(k,k',t)$, j=1,2



Fermions

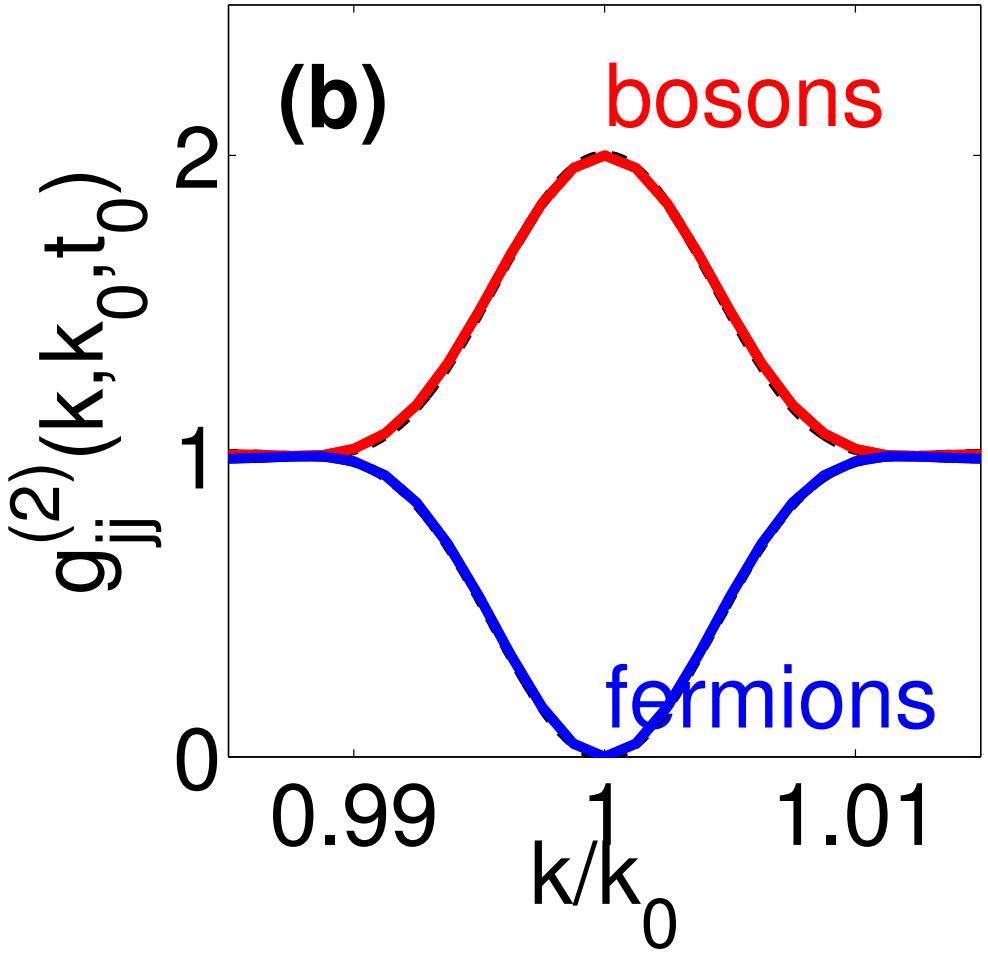
Figure 2 | Normalized correlation functions for ^{4}He* (bosons) in the upper plot, and ^{3}He* (fermions) in the lower plot. Both functions are measured at the same cloud temperature (0.5 μK), and with identical trap parameters.

T. Jeltes *et al.*, Nature 445 (2007) 402.

See also: M. Henny *et al.*, Science 284, 296 (1999). For 'anti-bunching of electrons' in a solid state device.

Heisenberg equation (UMF)

(b) Collinear (CL) correlations due to particle statistics, (like Hanbury Brown and Twiss for photons).



We have derived an analytical asymptote (dashed lines), strictly valid for short times ($t/t_0 \ll 1$). But useful even for $t/t_0 \sim 1$ as here. Solid lines are from a numerical calculation at $t/t_0 = 0.5$.

$$g^{(2)}_{jj}(k,k',t) \simeq 1 \begin{matrix} + \\ - \end{matrix} \frac{9\pi}{2} \frac{\left(J_{3/2}\left[(k-k')R_{\mathrm{TF}}\right]\right)^2}{\left[(k-k')R_{\mathrm{TF}}\right]^3}$$

Gaussian Fermionic phase-space representation

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}\left[\hat{H},\hat{\rho}\right]$$ **Liouville eq. for the density operator.**

Use fermionic phase-space mappings (recipe), e.g.:

$$\hat{c}_i^\dagger \hat{c}_j \hat{\rho} \rightarrow \left[n_{ij} + \sum_{l,k} \left(-\frac{\partial}{\partial n_{lk}} \left\{ n_{lj}\bar{n}_{ik} + m_{li}^+ m_{jk} \right\} \right.\right.$$

$$\left.\left. -\frac{\partial}{\partial m_{lk}} \left\{ m_{lj}\bar{n}_{ik} + \bar{n}_{il} m_{jk} \right\} + \frac{\partial}{\partial m_{lk}^+} \left\{ n_{lj} m_{ik}^+ + m_{li}^+ n_{kj} \right\} \right) \right] P(\boldsymbol{\alpha})$$

To obtain a FPE, assumes fast decaying tails.

$$\frac{\partial}{\partial t} P(\vec{\lambda}) = \left[-\sum_j \frac{\partial}{\partial \lambda_j} A_j(\vec{\lambda}) + \frac{1}{2} \sum_{j,k} \frac{\partial^2}{\partial \lambda_j \partial \lambda_k} D_{ij}(\vec{\lambda}) \right] P(\vec{\lambda})$$

Transform to SDE

$$D = BB^T,$$

$$\dot{z}_j = A_j\left(\vec{z}\right) + \sum_k B_{j,k}\left(\vec{z}\right)\eta_k$$

Fermionic phase-space representation

$$\hat{H} = \hat{H}_0 - i\hbar\chi \int d\mathbf{x} \left(\hat{\Psi}_0^\dagger \hat{\Psi}_1 \hat{\Psi}_2 - \hat{\Psi}_2^\dagger \hat{\Psi}_1^\dagger \hat{\Psi}_0 \right)$$

Transform to Fourier space, assume a uniform field.

$$\widehat{H} = \hbar \sum\nolimits_{\mathbf{k},\sigma} \Delta_{\mathbf{k}} \hat{n}_{\mathbf{k},\sigma} - i\hbar\kappa \sum\nolimits_{\mathbf{k}} \left(\hat{a}_0^\dagger \hat{m}_{\mathbf{k}} - \hat{m}_{\mathbf{k}}^\dagger \hat{a}_0 \right)$$

Transform to FPE

Transform to SDE (compare PMFT)

$$D = BB^T,\ B = \left[\mathbf{B}^{(n_\mathbf{k})}, \mathbf{B}^{(m_\mathbf{k})}, \mathbf{B}^{(m_\mathbf{k}^+)}, \mathbf{B}^{(\alpha)}, \mathbf{B}^{(\alpha^+)} \right]^T$$

$$\begin{aligned}
&\partial_t P = 2i \sum\nolimits_{\mathbf{k}} \Delta_{\mathbf{k}} \left[\partial_{m_\mathbf{k}} m_\mathbf{k} - \partial_{m_\mathbf{k}^+} m_\mathbf{k}^+ \right] P \\
&+\kappa \sum\nolimits_{\mathbf{k}} \left[-\partial_{n_\mathbf{k}} \left(\beta^+ m_\mathbf{k} + \beta m_\mathbf{k}^+ \right) - \partial_{m_\mathbf{k}} \beta \left(1 - 2n_\mathbf{k} \right) \right. \\
&-\partial_{m_\mathbf{k}^+} \beta^+ \left(1 - 2n_\mathbf{k} \right) + \partial_\beta m_\mathbf{k} + \partial_{\beta^+} m_\mathbf{k}^+ \\
&+\partial_{n_\mathbf{k}} \partial_\beta n_\mathbf{k} m_\mathbf{k} + \partial_{n_\mathbf{k}} \partial_{\beta^+} n_\mathbf{k} m_\mathbf{k}^+ + \partial_{m_\mathbf{k}} \partial_\beta m_\mathbf{k}^2 \\
&\left. -\partial_{m_\mathbf{k}} \partial_{\beta^+} n_\mathbf{k}^2 - \partial_{m_\mathbf{k}^+} \partial_\beta n_\mathbf{k}^2 + \partial_{m_\mathbf{k}^+} \partial_{\beta^+} m_\mathbf{k}^{+2} \right] P.
\end{aligned}$$

$$\begin{aligned}
dn_\mathbf{k} &= \left(\alpha m_\mathbf{k}^+ + \alpha^+ m_\mathbf{k} \right) d\tau + N_0^{-1/2} \mathbf{B}^{(n_\mathbf{k})} \mathbf{dW}, \\
dm_\mathbf{k} &= \left[-2i\delta_\mathbf{k} m_\mathbf{k} + \alpha \left(1 - 2n_\mathbf{k} \right) \right] d\tau + N_0^{-1/2} \mathbf{B}^{(m_\mathbf{k})} \mathbf{dW}, \\
dm_\mathbf{k}^+ &= \left[2i\delta_\mathbf{k} m_\mathbf{k}^+ + \alpha^+ \left(1 - 2n_\mathbf{k} \right) \right] d\tau + N_0^{-1/2} \mathbf{B}^{(m_\mathbf{k}^+)} \mathbf{dW}, \\
d\alpha &= -\tfrac{1}{N_0} \textstyle\sum_\mathbf{k} m_\mathbf{k} d\tau + N_0^{-1/2} \mathbf{B}^{(\alpha)} \mathbf{dW}, \\
d\alpha^+ &= -\tfrac{1}{N_0} \textstyle\sum_\mathbf{k} m_\mathbf{k}^+ d\tau + N_0^{-1/2} \mathbf{B}^{(\alpha^+)} \mathbf{dW},
\end{aligned}$$

Fermionic phase-space representation

Stochastically sampled moments can be related to physical expectation values. For example, the first-order moments give:

$$\begin{cases} \langle n_{\mathbf{k}} \rangle_S &= \langle \hat{n}_{\mathbf{k}} \rangle = \langle \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle, \\ \langle m_{\mathbf{k}} \rangle_S &= \langle \hat{m}_{\mathbf{k}} \rangle = \langle \hat{b}_{\mathbf{k},1} \hat{b}_{-\mathbf{k},2} \rangle, \\ \langle \alpha \rangle_S &= \langle \hat{a}_0 \rangle / \sqrt{N_0}. \end{cases} \tag{6.10}$$

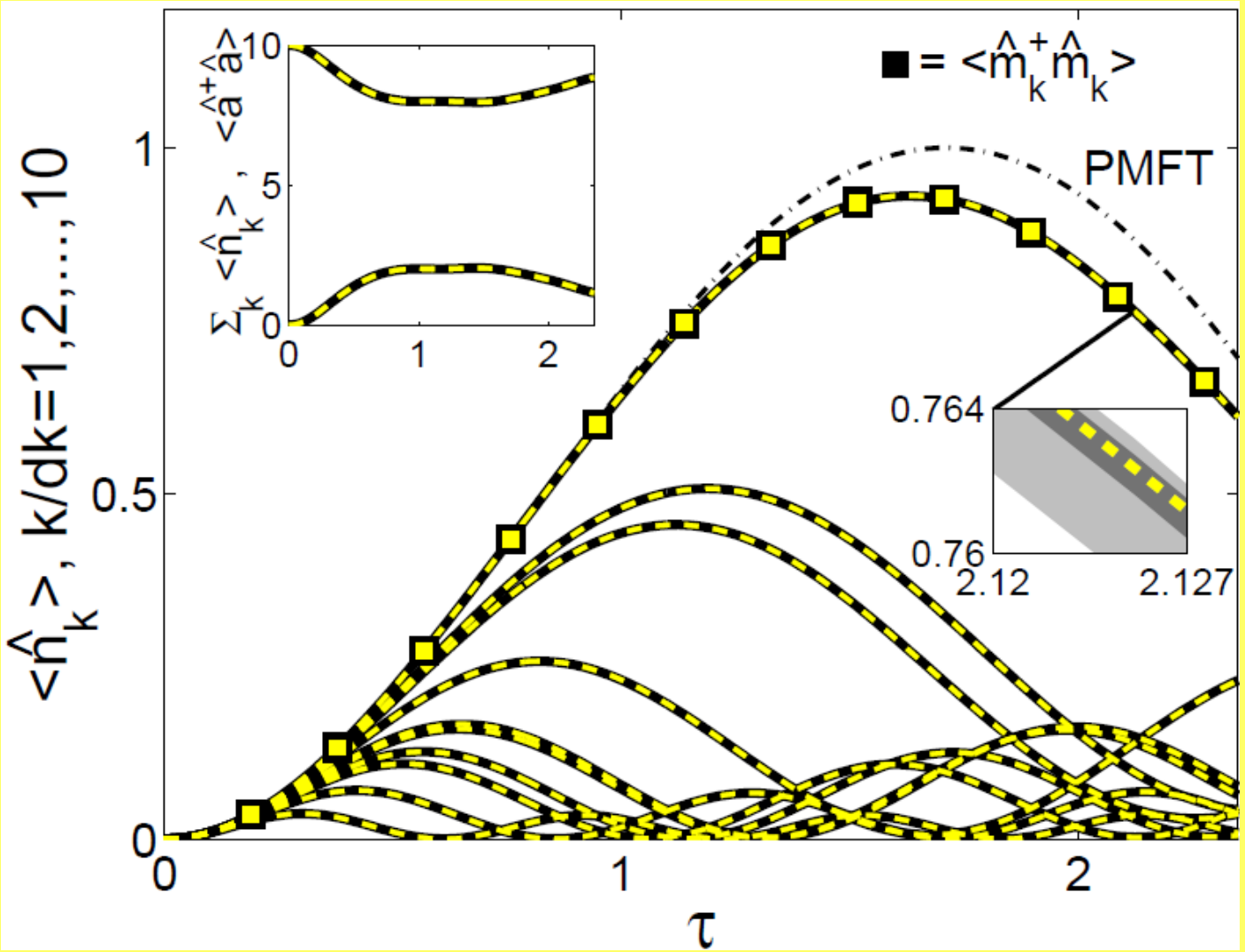
Normally ordered higher-order moments are obtained exactly by stochastic averages of a corresponding Wick decomposition [60, 94, 95], as in the following example

$$\langle m^{+}_{\mathbf{k}} m_{\mathbf{k}} \rangle_S + \langle n^2_{\mathbf{k}} \rangle_S = \langle \hat{m}^{\dagger}_{\mathbf{k}} \hat{m}_{\mathbf{k}} \rangle. \tag{6.11}$$

ALL! observables available, though only few first order moments are propagated in time.

Numerical results for molecular dissociation

Comparison of atomic mode occupations



We compare with the "number-base expansion" (C.I.)

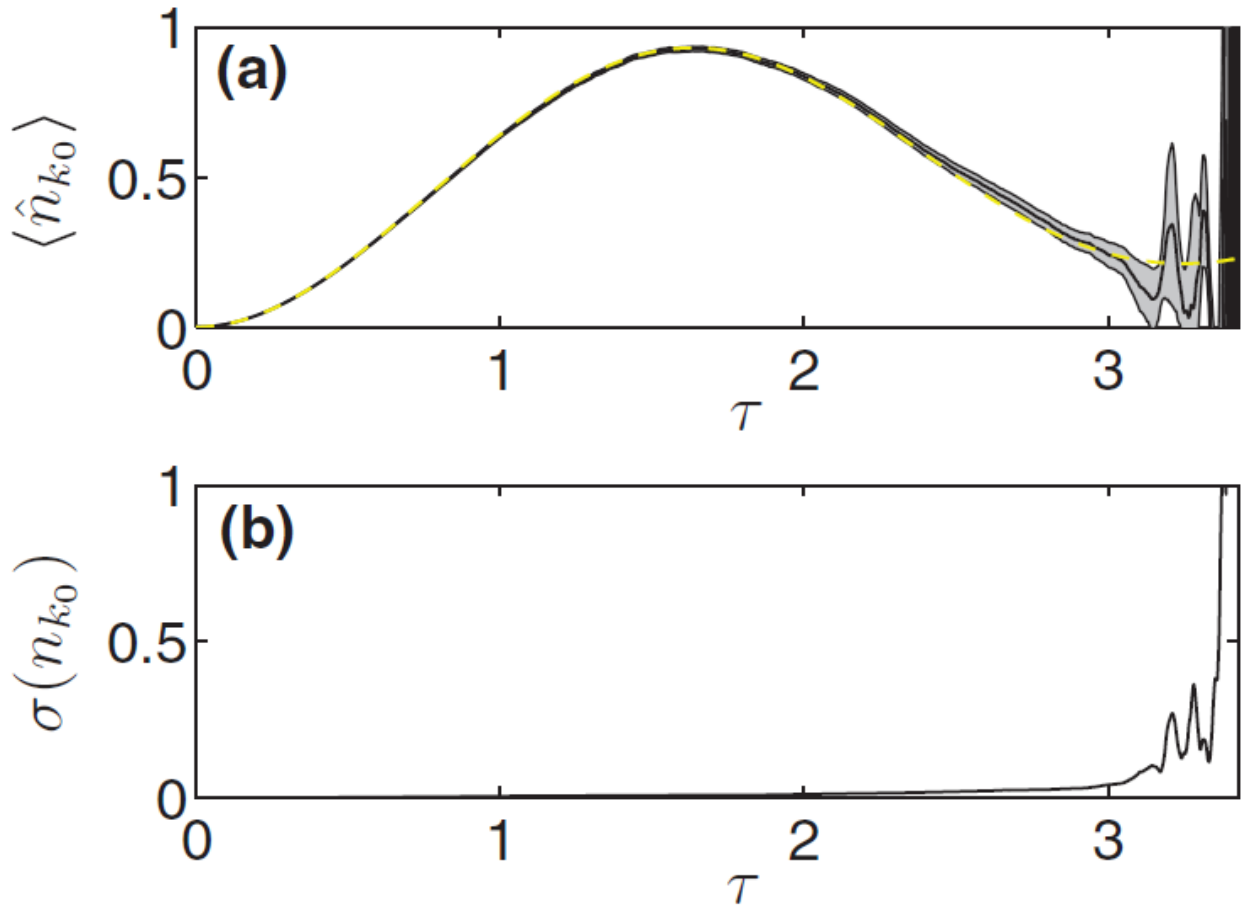
For few modes we can solve the full time-dependent Schrödinger equation ("in second quantization") for the mixed fermion-boson state.

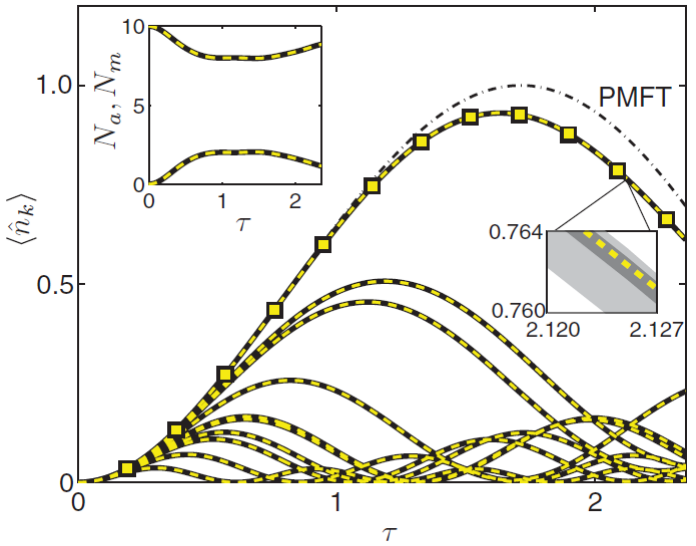
$$\Psi(\tau) = \sum_{j=1}^{2^M} \sum_{n=1}^{n_{\max}} c_{j,n} \left|\vec{n}_j\right\rangle \otimes |n\rangle = e^{-i\tau H} \Psi_0,\ H \in \mathbb{C}^d \times \mathbb{C}^d$$

Test system with M=10 modes, to compare with the phase-space method

$$d = 2^M n_{\max} \simeq 10^5$$

What about “spikes”?





Numerical results for molecular dissociation

Comparison of atomic mode occupations

- **Excellent agreement up to the spiking time.**
- **Deviations from mean-field results (PMFT).**
- **The limited simulation time is 'enough' here.**
- **Operator equality:** $\hat{m}_{\mathbf{k}}^{\dagger}\hat{m}_{\mathbf{k}}\,(=\hat{n}_{\mathbf{k},1}\hat{n}_{-\mathbf{k},2})=\hat{n}_{\mathbf{k}}$

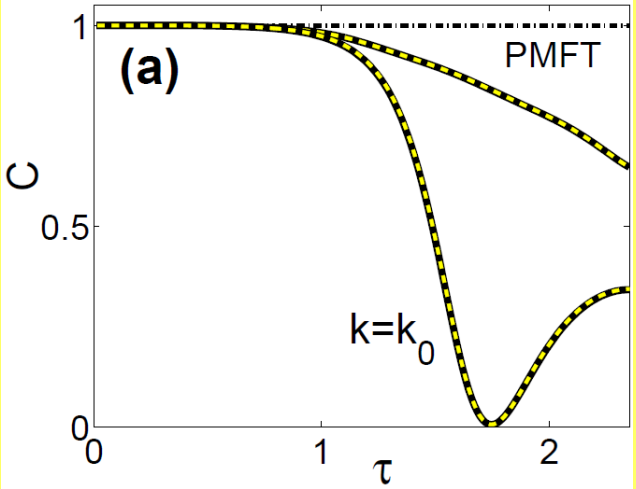
used to check stochastic averages: $\langle\hat{m}_{\mathbf{k}}^{\dagger}\hat{m}_{\mathbf{k}}\rangle=\langle m_{\mathbf{k}}^{+}m_{\mathbf{k}}\rangle_S+\langle n_{\mathbf{k}}^{2}\rangle_S$

Numerical results for molecular dissociation

Comparison of correlation coefficients C and W

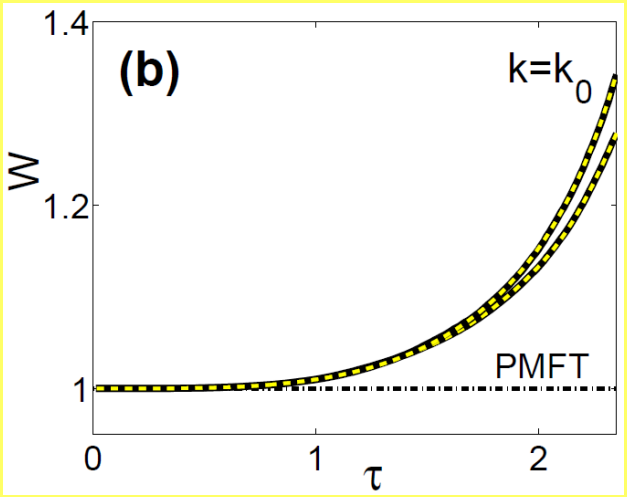
$$C = \sum_{\mathbf{k}} |\langle \hat{m}_{\mathbf{k}} \rangle|^2 \; / \; \sum_{\mathbf{k}} \left(\langle \hat{n}_{\mathbf{k}} \rangle - \langle \hat{n}_{\mathbf{k}} \rangle^2 \right)$$

Quantify deviations from PMFT



$$W = \sum_{\mathbf{k}} \langle \hat{m}^{\dagger}_{\mathbf{k}} \hat{m}_{\mathbf{k}} \rangle \; / \; \sum_{\mathbf{k}} \left(|\langle \hat{m}_{\mathbf{k}} \rangle|^2 + \langle \hat{n}_{\mathbf{k}} \rangle^2 \right)$$

Also quantify deviations from Wick's theorem

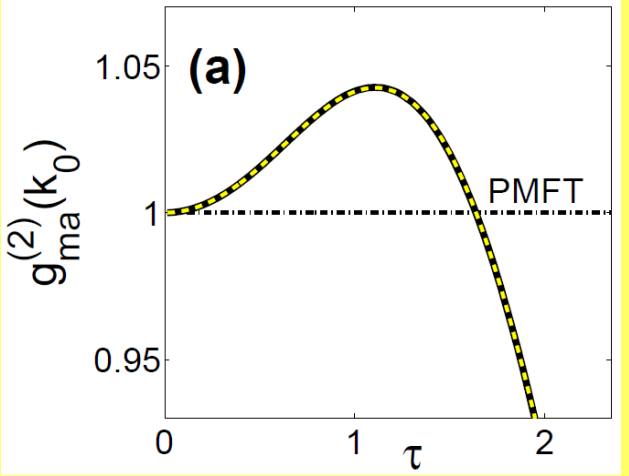


Numerical results for molecular dissociation

Comparison of molecular correlations

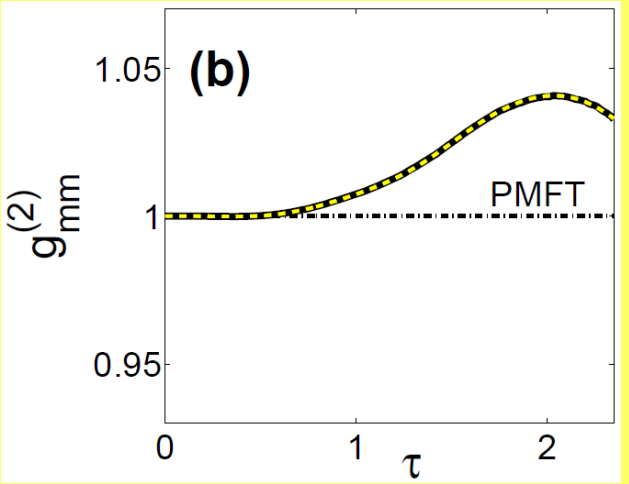
$$g^{(2)}_{ma}(\mathbf{k}) = \frac{\langle \hat{a}^\dagger \hat{a} \hat{n}_{\mathbf{k}} \rangle}{\langle \hat{a}^\dagger \hat{a} \rangle \langle \hat{n}_{\mathbf{k}} \rangle}$$

Molecule-atom correlation



$$g^{(2)}_{mm} = \frac{\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \rangle}{\langle \hat{a}^\dagger \hat{a} \rangle^2}$$

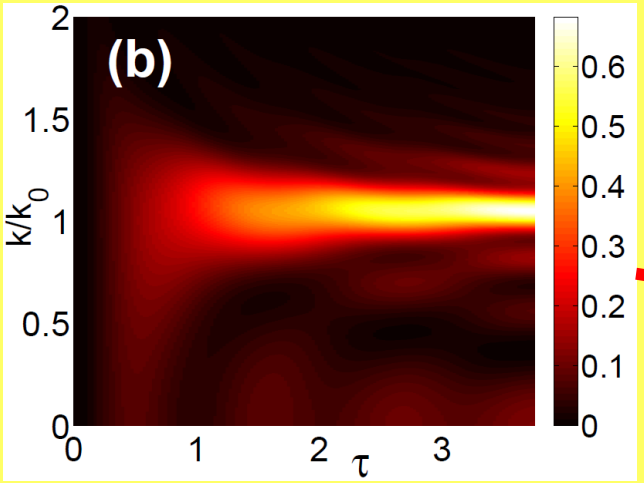
Glauber 2.nd order

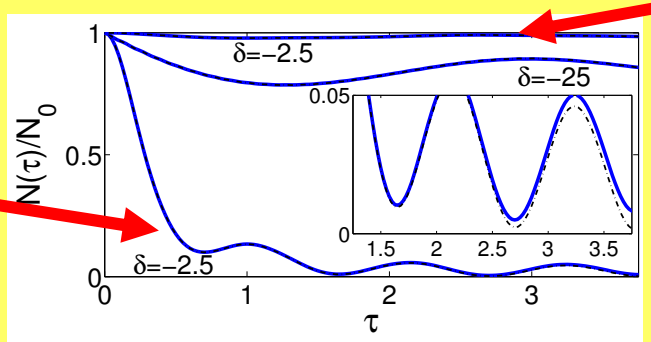


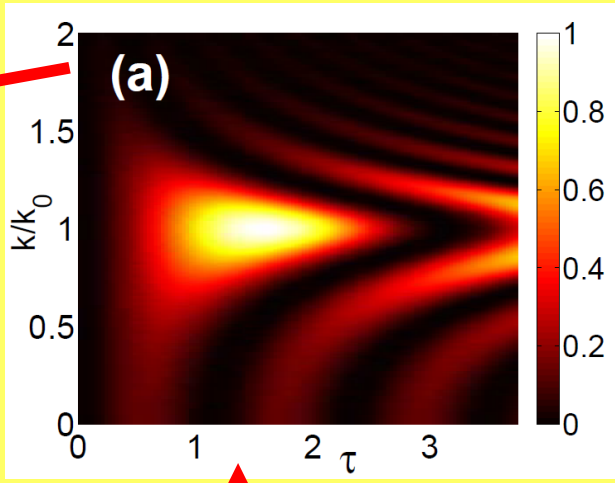
Application to molecular dissociation: Large systems

Multimode simulations with M=1000 atomic modes, Hilbert space dimension $d = 2^M \cdot n_{max} \gg 10^{300}$

The phase-space method handle this on an old PC







$$\sin^2(\sqrt{\delta_k^2+1}\,\tau)/(\delta_k^2+1)$$

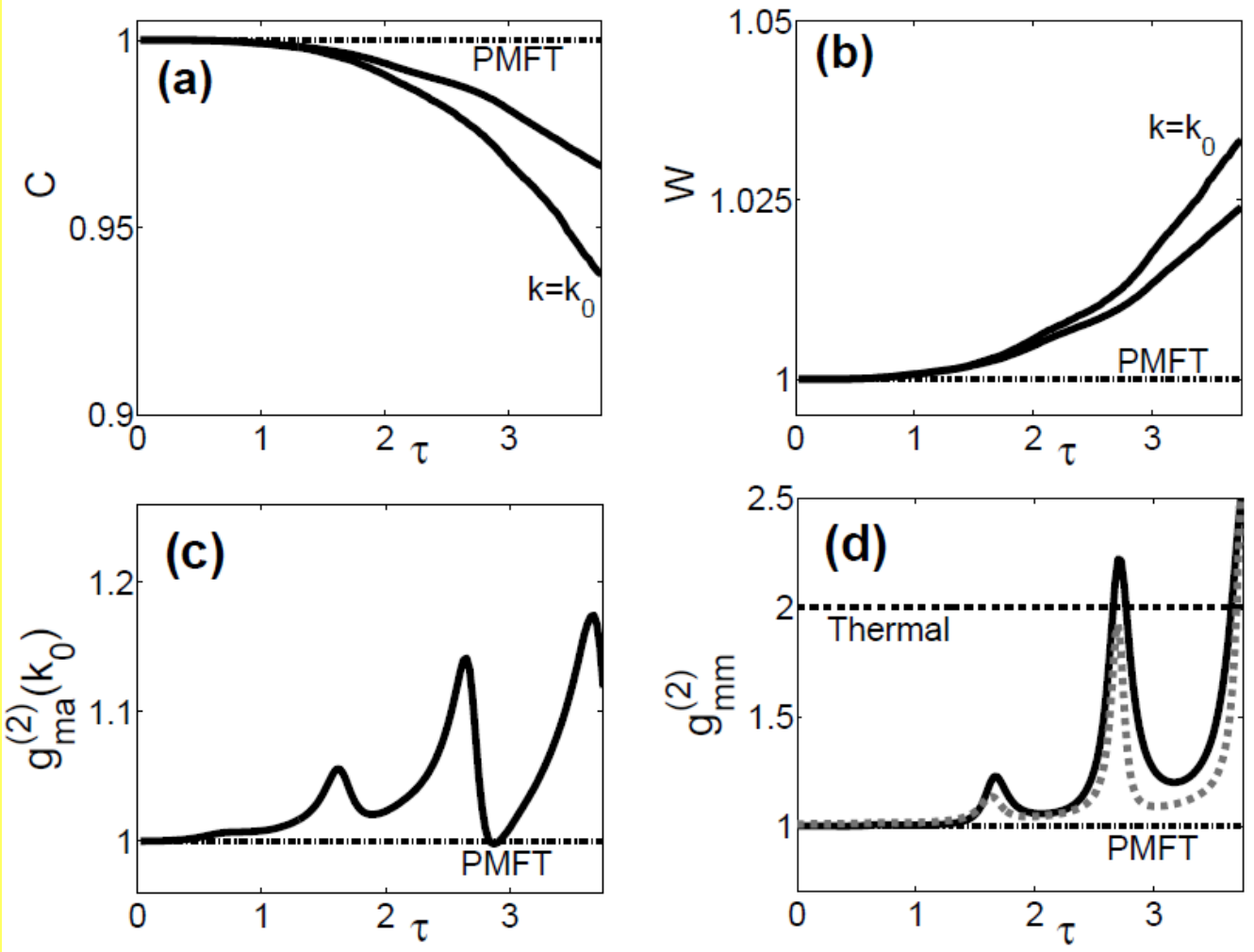
- **Deviations from PMFT**
- **Limited simulation time (enough for this application)**

Application to molecular dissociation: Large systems

Multimode simulations with M=1000 atomic modes

The phase-space method reveals correlations not available within PMFT .

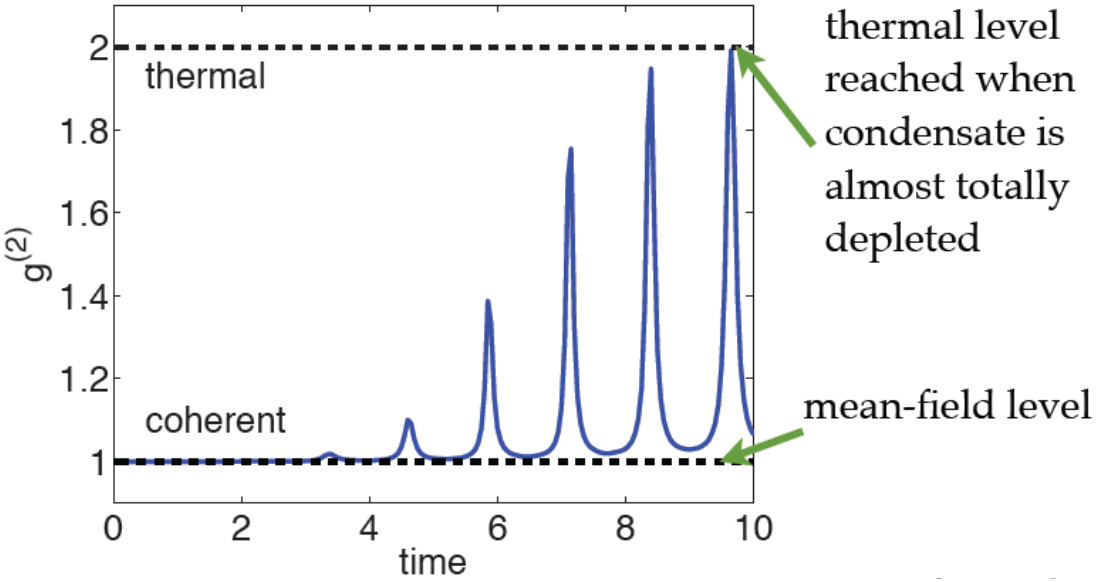
(However, PMFT performs well for atom numbers and densities.)



What about higher dimensions?

Dynamics in 2 dimensions

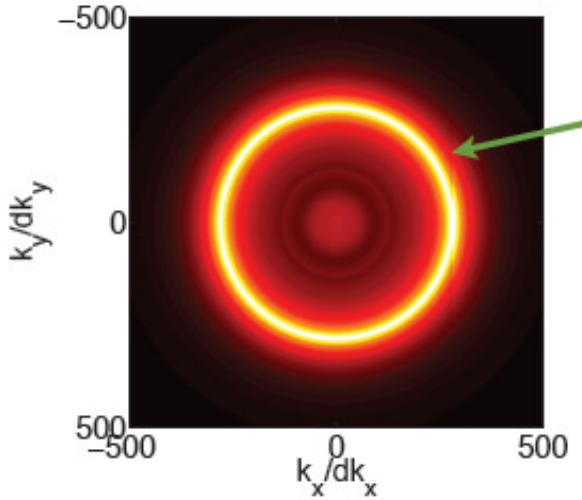
Molecular correlations



thermal level reached when condensate is almost totally depleted

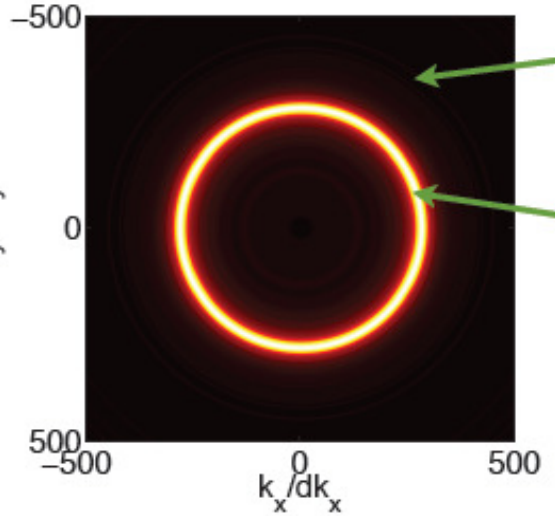
mean-field level

Atomic momentum distribution at time = 10:



atom density peaks around resonant ring

Atomic correlations W at time = 10:



black is mean-field level

non-mean-field correlations strongest on resonant ring

2D example with:
80.000 molecules and
1.000.000 atomic modes

Fermionic phase-space representation

Exploring gauge freedoms to extend simulation time

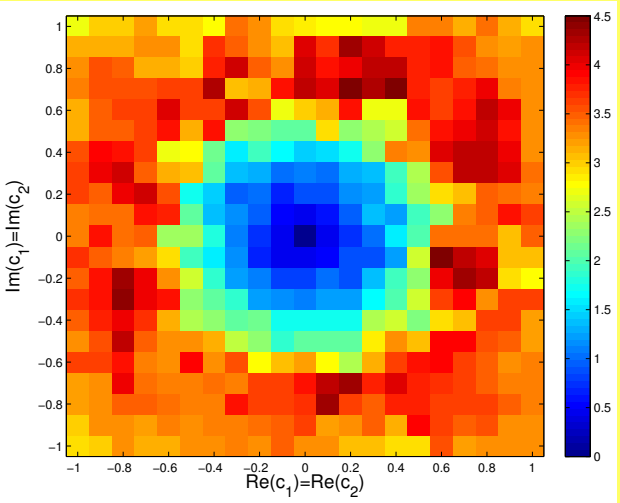
$$\widehat{H} = \hbar \sum_{\mathbf{k},\sigma} \Delta_{\mathbf{k}} \hat{n}_{\mathbf{k},\sigma} - i\hbar\kappa \sum_{\mathbf{k}} \left(\hat{a}^{\dagger} \hat{m}_{\mathbf{k}} - \hat{m}_{\mathbf{k}}^{\dagger} \hat{a} \right)$$

$$\begin{aligned}
\dot{n}_{\mathbf{k}} &= \alpha m_{\mathbf{k}}^{+} + \alpha^{+} m_{\mathbf{k}} + N_0^{-1/2} n_{\mathbf{k}} \left(m_{\mathbf{k}} \zeta_1^{*} + m_{\mathbf{k}}^{+} \zeta_2^{*} \right) \\
\dot{m}_{\mathbf{k}} &= -2i\delta_{\mathbf{k}} m_{\mathbf{k}} + \alpha \left(1 - 2n_{\mathbf{k}} \right) + N_0^{-1/2} \left(m_{\mathbf{k}}^{2} \zeta_1^{*} - n_{\mathbf{k}}^{2} \zeta_2^{*} \right) \\
\dot{m}_{\mathbf{k}}^{+} &= 2i\delta_{\mathbf{k}} m_{\mathbf{k}}^{+} + \alpha^{+} \left(1 - 2n_{\mathbf{k}} \right) + N_0^{-1/2} \left(m_{\mathbf{k}}^{+2} \zeta_2^{*} - n_{\mathbf{k}}^{2} \zeta_1^{*} \right) \\
\dot{\alpha} &= -\tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}} + N_0^{-1/2} \zeta_1 \\
\dot{\alpha}^{+} &= -\tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}}^{+} + N_0^{-1/2} \zeta_2,
\end{aligned}$$

$$\begin{aligned}
\dot{n}_{\mathbf{k}} &= \alpha m_{\mathbf{k}}^{+} + \alpha^{+} m_{\mathbf{k}} + N_0^{-1/2} n_{\mathbf{k}} \left(\zeta_{\mathbf{k}}^{(1)*} + \zeta_{\mathbf{k}}^{(2)*} \right) \\
\dot{m}_{\mathbf{k}} &= -2i\delta_{\mathbf{k}} m_{\mathbf{k}} + \alpha \left(1 - 2n_{\mathbf{k}} \right) + N_0^{-1/2} \left(m_{\mathbf{k}} \zeta_{\mathbf{k}}^{(1)*} - n_{\mathbf{k}} \zeta_{\mathbf{k}}^{(4)*} \right) \\
\dot{m}_{\mathbf{k}}^{+} &= 2i\delta_{\mathbf{k}} m_{\mathbf{k}}^{+} + \alpha^{+} \left(1 - 2n_{\mathbf{k}} \right) + N_0^{-1/2} \left(m_{\mathbf{k}}^{+} \zeta_{\mathbf{k}}^{(2)*} - n_{\mathbf{k}} \zeta_{\mathbf{k}}^{(3)*} \right) \\
\dot{\alpha} &= -1.5 \tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}} + N_0^{-1/2} \sum_{\mathbf{k}} \left(m_{\mathbf{k}} \zeta_{\mathbf{k}}^{(1)} + n_{\mathbf{k}} \zeta_{\mathbf{k}}^{(3)} \right) \\
\dot{\alpha}^{+} &= -1.5 \tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}}^{+} + N_0^{-1/2} \sum_{\mathbf{k}} \left(m_{\mathbf{k}}^{+} \zeta_{\mathbf{k}}^{(2)} + n_{\mathbf{k}} \zeta_{\mathbf{k}}^{(4)} \right),
\end{aligned}$$

… ? !

As a first step we have optimized a ‘complex number’ diffusion gauge



Extend simulation time with >50%

Fermionic phase-space representation

Examples of different realizations of the stochastic terms

$$
\begin{aligned}
dn_{\mathbf{k}} &= \left(\alpha m_{\mathbf{k}}^{+} + \alpha^{+} m_{\mathbf{k}}\right) d\tau + N_0^{-1/2} \mathbf{B}^{(n_{\mathbf{k}})} \mathbf{dW}, \\
dm_{\mathbf{k}} &= \left[-2i\delta_{\mathbf{k}} m_{\mathbf{k}} + \alpha\left(1 - 2n_{\mathbf{k}}\right)\right] d\tau + N_0^{-1/2} \mathbf{B}^{(m_{\mathbf{k}})} \mathbf{dW}, \\
dm_{\mathbf{k}}^{+} &= \left[2i\delta_{\mathbf{k}} m_{\mathbf{k}}^{+} + \alpha^{+}\left(1 - 2n_{\mathbf{k}}\right)\right] d\tau + N_0^{-1/2} \mathbf{B}^{(m_{\mathbf{k}}^{+})} \mathbf{dW}, \\
d\alpha &= -\tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}} d\tau + N_0^{-1/2} \mathbf{B}^{(\alpha)} \mathbf{dW}, \\
d\alpha^{+} &= -\tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}}^{+} d\tau + N_0^{-1/2} \mathbf{B}^{(\alpha^{+})} \mathbf{dW},
\end{aligned}
\qquad
D = BB^{T},\ B = \left[\ \mathbf{B}^{(n_{\mathbf{k}})}, \mathbf{B}^{(m_{\mathbf{k}})}, \mathbf{B}^{(m_{\mathbf{k}}^{+})}, \mathbf{B}^{(\alpha)}, \mathbf{B}^{(\alpha^{+})}\ \right]^{T}
$$

$$
B_I = \begin{bmatrix}
n_{\mathbf{k}} m_{\mathbf{k}} & -i n_{\mathbf{k}} m_{\mathbf{k}} & n_{\mathbf{k}} m_{\mathbf{k}}^{+} & -i n_{\mathbf{k}} m_{\mathbf{k}}^{+} \\
m_{\mathbf{k}}^{2} & -i m_{\mathbf{k}}^{2} & -n_{\mathbf{k}}^{2} & i n_{\mathbf{k}}^{2} \\
-n_{\mathbf{k}}^{2} & i n_{\mathbf{k}}^{2} & m_{\mathbf{k}}^{+2} & -i m_{\mathbf{k}}^{+2} \\
1 & i & 0 & 0 \\
0 & 0 & 1 & i
\end{bmatrix}
\qquad
B_{II} = \begin{bmatrix}
n_{\mathbf{k}} & -i n_{\mathbf{k}} & n_{\mathbf{k}} & -i n_{\mathbf{k}} & 0 & 0 & 0 & 0 \\
m_{\mathbf{k}} & -i m_{\mathbf{k}} & 0 & 0 & 0 & 0 & -n_{\mathbf{k}} & i n_{\mathbf{k}} \\
0 & 0 & m_{\mathbf{k}}^{+} & -i m_{\mathbf{k}}^{+} & -n_{\mathbf{k}} & i n_{\mathbf{k}} & 0 & 0 \\
m_{\mathbf{k}} & i m_{\mathbf{k}} & 0 & 0 & n_{\mathbf{k}} & i n_{\mathbf{k}} & 0 & 0 \\
0 & 0 & m_{\mathbf{k}}^{+} & i m_{\mathbf{k}}^{+} & 0 & 0 & n_{\mathbf{k}} & i n_{\mathbf{k}}
\end{bmatrix}
$$

$$
\mathbf{dW}_I = \left[\ dw_1 \quad dw_2 \quad dw_3 \quad dw_4\ \right]^{T} / \sqrt{2}.
\qquad
\mathbf{dW}_{II} = \left[\ dw_{1,\mathbf{k}} \quad dw_{2,\mathbf{k}} \quad \ldots \quad dw_{8,\mathbf{k}}\ \right]^{T} / \sqrt{2}
$$

Note that if the stochastic terms are neglected we obtain PMFT!

Fermionic phase-space representation

Conserved quantities:

$$F_{\mathbf{k}} \equiv \left\langle \widehat{m}_{\mathbf{k}}^{\dagger} \widehat{m}_{\mathbf{k}} \right\rangle - \langle \widehat{n}_{\mathbf{k}} \rangle$$

$$E \equiv \langle \hat{H} \rangle / 2\hbar|\Delta|$$

$$N \equiv \left(2\langle \hat{a}_0^{\dagger} \hat{a}_0 \rangle + \sum_{\mathbf{k},\sigma} \langle \hat{n}_{\mathbf{k},\sigma} \rangle \right) / 2N_0$$

Stochastic implementation:

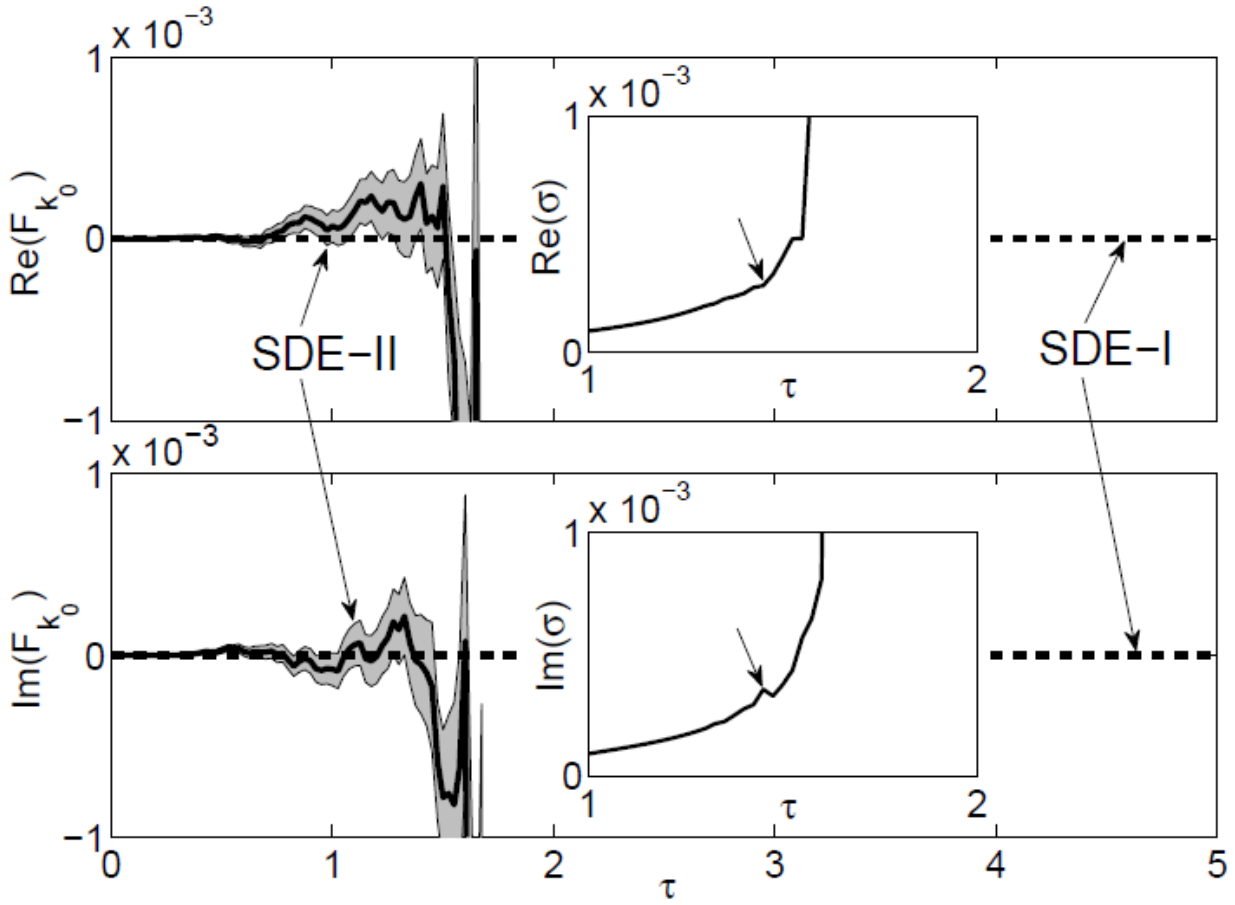
$$F_{\mathbf{k}} = \langle m_{\mathbf{k}}^{+} m_{\mathbf{k}} + n_{\mathbf{k}}^2 - n_{\mathbf{k}} \rangle_S,$$

$$E = \frac{1}{|\Delta|} \sum_{\mathbf{k}} \langle \Delta_{\mathbf{k}} n_{\mathbf{k}} - i \frac{\kappa \sqrt{N_0}}{2} \left(\alpha^{+} m_{\mathbf{k}} - \alpha m_{\mathbf{k}}^{+} \right) \rangle_S,$$

$$N = \left\langle \alpha^{+} \alpha \right\rangle_S + \frac{1}{N_0} \sum_{\mathbf{k}} \left\langle n_{\mathbf{k}} \right\rangle_S .$$

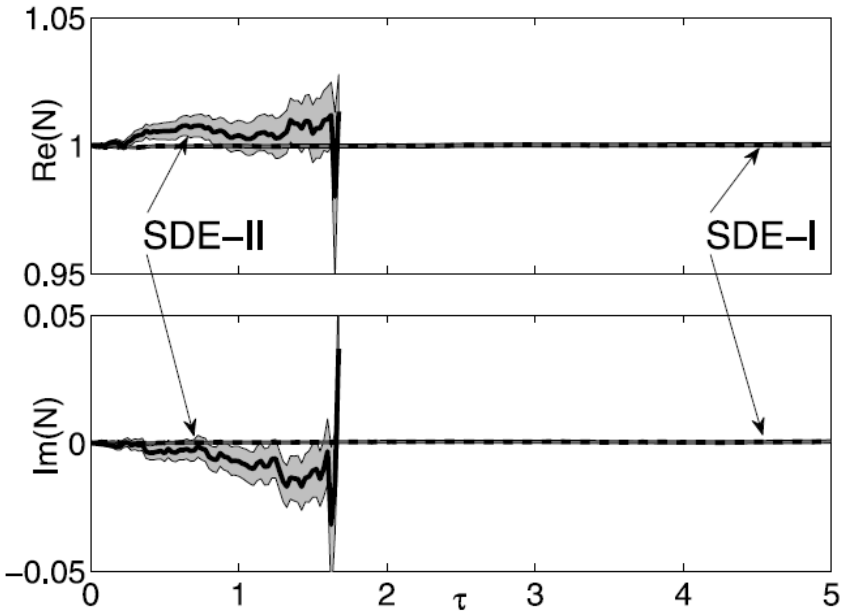
Fermionic phase-space representation

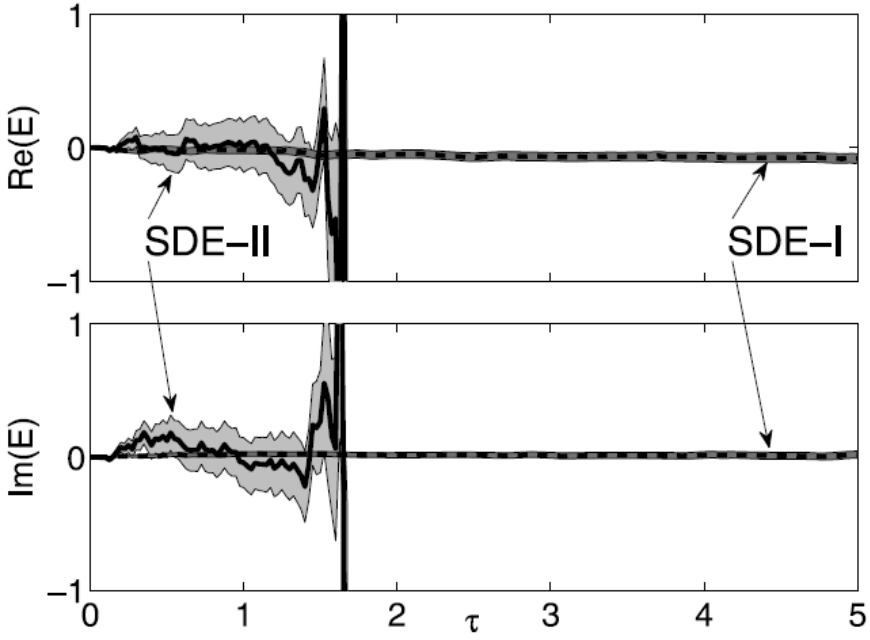
eters. In addition, we have shown that the simulation of conserved quantities can have qualitatively different behaviour for different gauges. The conserved quantities thus provide a check on numerical implementation and allow the performance of different gauges to be benchmarked.



Fermionic phase-space representation

For the energy and particle number, the average is still constant within the sampling error, as shown in Figs. 2 and 3.





What is the problem II ?

Rahav S and Mukamel S 2009 *Phys. Rev.* B **79** 165103

General two-Body interaction (e.g. Coulomb)

$$\hat{\mathcal{H}} = \sum_{\alpha\beta} t_{\alpha\beta}\hat{c}^{\dagger}_{\alpha}\hat{c}_{\beta} + \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}\hat{c}^{\dagger}_{\alpha}\hat{c}^{\dagger}_{\beta}\hat{c}_{\gamma}\hat{c}_{\delta}. \qquad (2)$$

The indices $\alpha, \beta, \gamma, \delta$ denote an orthogonal one particle basis of spin orbitals. The creation and annihilation operators satisfy the Fermi anticommutation rule,

$$\hat{c}^{\dagger}_{\alpha}\hat{c}_{\beta} + \hat{c}_{\beta}\hat{c}^{\dagger}_{\alpha} = \delta_{\alpha\beta}. \qquad (3)$$

Physicists playground (fermionic Hubbard model)

$$\widehat{H} = -J\hbar \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{j},\sigma} + U\hbar \sum_{\mathbf{j}} \hat{n}_{\mathbf{j},\uparrow}\hat{n}_{\mathbf{j},\downarrow} + \hbar \sum_{\mathbf{j},\sigma} V_{\mathbf{j},\sigma}\hat{n}_{\mathbf{j},\sigma}$$

Work in progress: Hubbard model

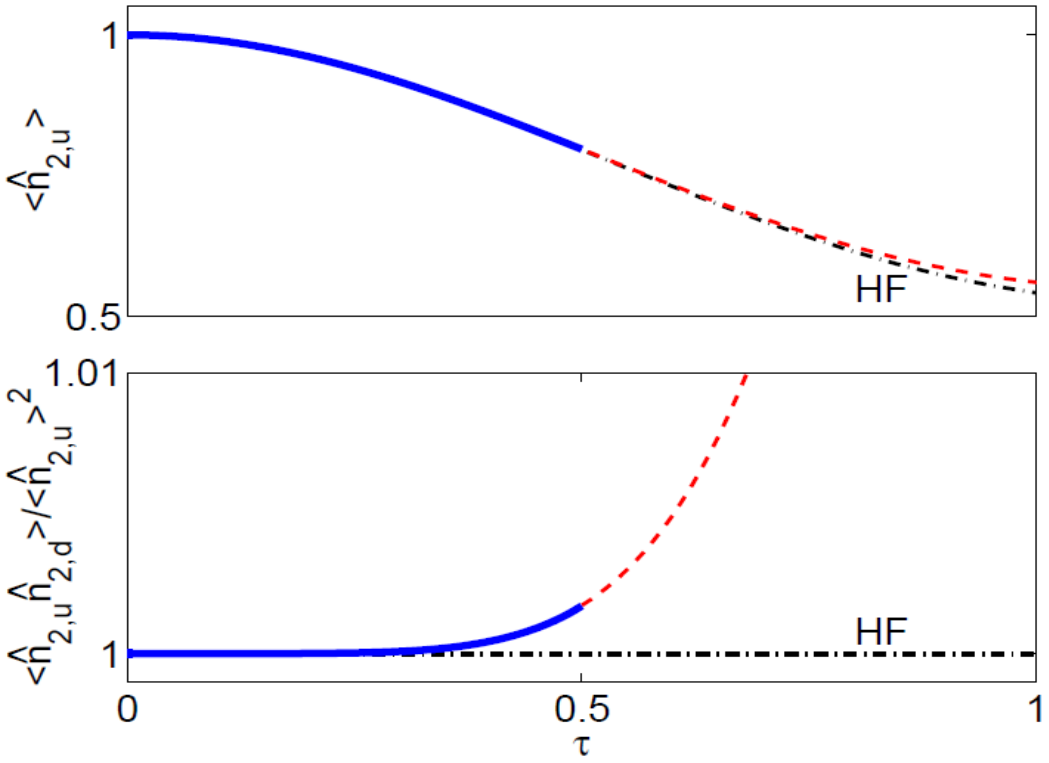
To investigate how the phase-space method works for fermionic systems with atom-atom interactions, we focus on the Hamiltonian

$$\widehat{H} = -J\hbar \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{j},\sigma} + U\hbar \sum_{\mathbf{j}} \hat{n}_{\mathbf{j},\uparrow}\hat{n}_{\mathbf{j},\downarrow} + \hbar \sum_{\mathbf{j},\sigma} V_{\mathbf{j},\sigma}\hat{n}_{\mathbf{j},\sigma}. \qquad (6.21)$$

Gaussian Phase-Space representation

$$\dot{\mathbf{n}}_u = -i\left(\mathbf{n}_u\mathbf{A}_u - \mathbf{A}_u\mathbf{n}_u\right) + \sqrt{-iU}\,\mathbf{n}_u\zeta^{(1)}\bar{\mathbf{n}}_u + \sqrt{iU}\,\bar{\mathbf{n}}_u\zeta^{(2)}\mathbf{n}_u$$
$$\dot{\mathbf{n}}_d = -i\left(\mathbf{n}_d\mathbf{A}_d - \mathbf{A}_d\mathbf{n}_d\right) + \sqrt{-iU}\,\mathbf{n}_d\zeta^{(1)*}\bar{\mathbf{n}}_d + \sqrt{iU}\,\bar{\mathbf{n}}_d\zeta^{(2)*}\mathbf{n}_d.$$

Numerical simulations of the SDEs



Correct results (--CI), limited simulation time!

References I:

Gaussian representation for fermions

Gaussian phase-space representations for fermions.
J. Corney and P. Drummond, Phys. Rev. B **73**, 125112 (2006), arXiv:cond-mat/0411712v3 [cond-mat.other]

Gaussian operator bases for correlated fermions.
J. Corney and P. Drummond, J. Phys. A: Math. Gen. **39** (2006) 269-297 , arXiv:quant-ph/0511007v1

Gaussian quantum Monte Carlo methods for fermions.
J. Corney and P. Drummond, Phys. Rev. Lett. **93**, 260401 (2004), arXiv:quant-ph/0404052v2

Gauges etc.

Stochastic simulations of fermionic dynamics with phase-space representations.
M. Ögren, K. V. Kheruntsyan and J. F. Corney, Computer Physics Communications (2010), arXiv:1008.0970v1 [physics.comp-ph] Computer Physics Communications **182,** 1999 (2011).

P. Corboz, M. Ögren, K. Kheruntsyan and J. Corney, bookchapter: ”Phase-space methods for fermions”, in Quantum Gases: Finite Temperature and Non-Equilibrium Dynamics, Imperial College Press London (2013). ISBN-10: 1848168101.

References II:

Fermi Hubbard model, symmetry projection

Systematic errors in Gaussian Quantum Monte Carlo and a systematic study of the symmetry projection method.
P. Corboz *et. al.*, Phys. Rev. B **77**, 085108 (2008), arXiv:0707.4394v2 [cond-mat.str-el]

Gaussian-Basis Monte Carlo Method for Numerical Study on Ground States of Itinerant and Strongly Correlated Electron Systems.
T. Aimi and M. Imada, J. Phys. Soc. Jpn. **76** (2007) 084709, arXiv:0704.3792v1 [cond-mat.str-el]

Symmetry projection schemes for Gaussian Monte Carlo methods.
F. F. Assaad *et. al.*, Phys. Rev. B **72**, 224518 (2005), arXiv:cond-mat/0509149v1 [cond-mat.str-el]

Applications

First-principles quantum dynamics for fermions: application to molecular dissociation.
M. Ögren, K. V. Kheruntsyan and J. F. Corney
Preprint (2009), (arXiv:0910.4440v2 [cond-mat.quant-gas])

EPL **92**, 36003 (2010).

Gaussian phase-space representation of Fermion dynamics; Beyond the time-dependent-Hartree-Fock approximation
S. Rahav and S. Mukamel, Phys. Rev. B **79**, 165103 (2009), arXiv:0902.3227v2 [cond-mat.other]

Does Simple Two-Dimensional Hubbard Model Account for High-Tc Superconductivity in Copper Oxides?
T. Aimi and M. Imada, J. Phys. Soc. Jpn. **76** (2007) 113708, arXiv:0708.3416v1 [cond-mat.str-el]

Fermionic coherent states

K. E. Cahill and R. J. Glauber, Phys. Rev. A **59** 1538 (1999)

Fermi sign problem

Computational complexity and fundamental limitations to fermionic quantum Monte Carlo simulations.
M. Troyer and U. J. Wiese, Phys. Rev. Lett. **94**, 170201 (2005), arXiv:cond-mat/0408370v1 [cond-

Summary of fermionic phase-space results

* **First dynamical multi-mode phase-space simulation for fermionic atoms from dissociation successful!**

* **Large deviations from mean-field methods (PMFT) for some correlations. Justify PMFT for atom numbers and densities if the molecular depletion is small.**

* **Diffusion gauges change the numerical performance and can qualitatively change the behaviour of conserved quantities.**

Thank you!