Fermionic phase-space method for many-body dynamics: Application to molecular dissociation

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Motivation

Simulations of interacting quantum many-body systems is a long standing problem!

Existing methods: time-dependent (TD) density functional theory (DFT) and matrix product state (MPS) based algorithms.

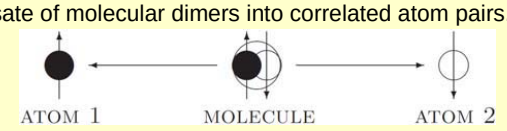
Challenges: (1) beyond few particles; (2) strongly correlated systems; (3) higher dimensional systems (D>1).

Phase space stochastic methods for bosons – long history of successful applications to real-time dynamics and ground-state (equilibrium) calculations.

Phase space stochastic methods for fermions is a new development; tested so far only for the *ground-state* of the Hubbard model [1,2].

Model system

As a first multi-mode *dynamical* application of the fermionic stochastic method we study dissociation of a Bose-Einstein condensate of molecular dimers into correlated atom pairs.



This is an atom optics analogue of parametric down-conversion with photons;

Down-conversion has been pivotal in the advancement of quantum optics; molecular dissociation may play a similar role in *quantum-atom optics*

Model Hamiltonian:

$$\hat{H} = \hat{H}_0 - i\hbar\chi_D \int d\mathbf{x} \left(\hat{\Psi}_0^\dagger \hat{\Psi}_\downarrow \hat{\Psi}_\uparrow - \hat{\Psi}_\downarrow^\dagger \hat{\Psi}_\uparrow^\dagger \hat{\Psi}_0 \right)$$

We study atom-atom, molecule-atom ,and molecule-molecule-correlations for molecules made of fermionic atoms

Our results go beyond the predictions of existing approximate methods (undepleted molecular field and the pairing mean-field method [3,4]).

Implementation via stochastic ODEs

For real-time dynamic we want to solve the Liouville equation.

The density operator is expanded in a continuous Gaussian operator base [1]; the Liouville equation is transformed into a Fokker-Planck equation, which in turn is transformed into a set of stochastic differential equations.

As an example, we consider a uniform molecular field in 1D

$$\hat{H} = \hbar \sum_{k,\sigma} \Delta_k \hat{n}_{k,\sigma} - i\hbar\kappa \sum_k \left(\hat{a}^\dagger \hat{b}_{\uparrow,k} \hat{b}_{\downarrow,-k} - \hat{b}_{\downarrow,-k}^\dagger \hat{b}_{\uparrow,k}^\dagger \hat{a} \right)$$

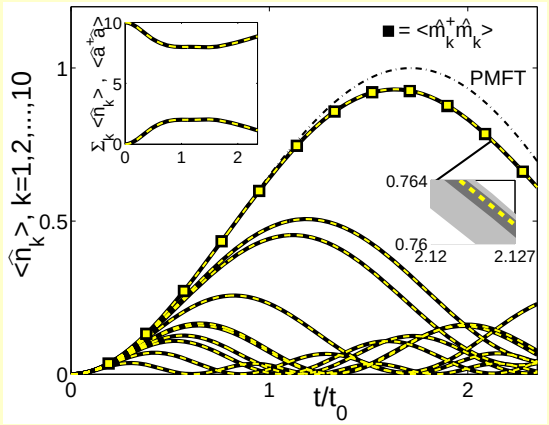
In practice, the dynamics is simulated via stochastic ODEs like e.g.:

$$\begin{aligned}
\dot{m}_{\mathbf{k}} &= \alpha m_{\mathbf{k}}^+ + \alpha^+ m_{\mathbf{k}} + N_0^{-1/4} n_{\mathbf{k}} \left(m_{\mathbf{k}} \zeta_1^* + m_{\mathbf{k}}^+ \zeta_2^* \right) \\
\dot{n}_{\mathbf{k}} &= -2i\delta_{\mathbf{k}} m_{\mathbf{k}} + \alpha \left(1 - 2n_{\mathbf{k}} \right) + N_0^{-1/4} \left(m_{\mathbf{k}}^2 \zeta_1^* - n_{\mathbf{k}}^2 \zeta_2^* \right) \\
\dot{m}_{\mathbf{k}}^+ &= 2i\delta_{\mathbf{k}} m_{\mathbf{k}}^+ + \alpha^+ \left(1 - 2n_{\mathbf{k}} \right) + N_0^{-1/4} \left(-n_{\mathbf{k}}^2 \zeta_1^* + m_{\mathbf{k}}^{+2} \zeta_2^* \right) \\
\dot{\alpha} &= -\tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}} + N_0^{-3/4} \zeta_1 \\
\dot{\alpha}^+ &= -\tfrac{1}{N_0} \textstyle\sum_{\mathbf{k}} m_{\mathbf{k}}^+ + N_0^{-3/4} \zeta_2 .
\end{aligned}$$

Averages over stochastic c-fields approach true quantum mechanical expectationvalues of operators in the limit of many realisations of the SDEs.

Few-mode system: test case

As a test example, we first compare the stochastic method for 10 molecules and 10 atomic modes with the solution to the Schrödinger equation in matrix representation.

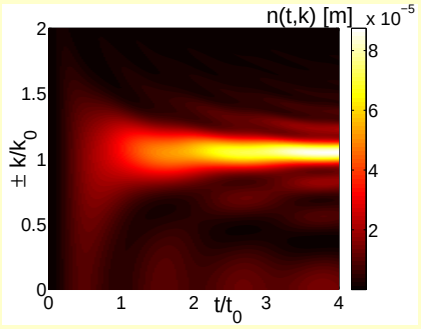


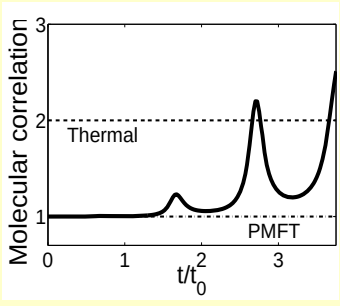
Excellent agreement (including for higher-order correlations) up to a certain simulation time where stochastic sampling problems occur. Sampling errors can be reduced by 'stochastic gauges'.

Results for a multi-mode system

Challenge: simulate a many-body system with 100 molecules and 1000 momentum modes (can not be done using Schrödinger's equation)

Can be done with the stochastic method on a standard PC!





The strongly depleted molecular field develops highly nontrivial pair correlation

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

Coherence is lost; the pairing mean-field theory (PMFT) breaks down.

Future work

- Treat non-uniform molecular condensates and higher dimensions
- Include atom-atom, molecule-atom and molecule-molecule s-wave scattering interactions
- Optimise 'stochastic gauges' to extend useful simulation time

References

[1] J. F. Corney and P. D. Drummond, Phys. Rev. B **73**, (2006).
[2] P. Corboz *et al*., Phys. Rev. B **77**, 085108 (2008).
[3] M. J. Davis *et al*., Phys. Rev. A **77**, 023617 (2008).
[4] M. Ögren and K. V. Kheruntsyan, Phys. Rev. A **78**, (2008).