Exact Quantum Dynamics of Fermionic systems

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The physics of interacting fermions is the basis of many of the most important phenomena in condensed matter physics, ultracold gases, and quantum chemistry. A fundamental issue is how the microscopic interactions at the quantum level give rise to collective and emergent effects in many-body systems. Ultracold quantum gases provide an ideal platform on which to explore such issues, through highly controllable implementations of analogue many-body systems for which the dynamical evolution and correlations are directly accessible. In order to make predictions from the underlying theory, to validate the potential quantum emulators, or to benchmark approximate approaches, a numerical simulation of the exact real-time dynamics is required.

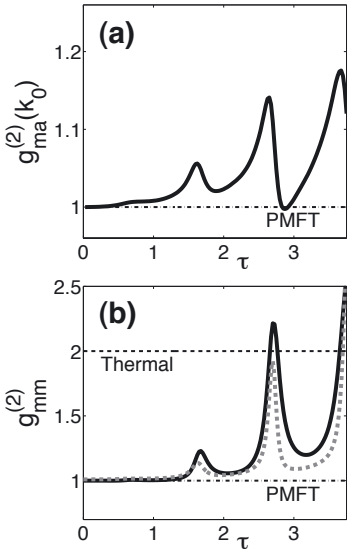

Fig. 1: Dynamical growth of second-order correlations: (a) Atom-molecule and (b) molecule-molecule correlations. Solid lines: exact, phase-space result; dot-dashed lines: pairing mean-field result; thick dashes: approximate semiclassical result.

To this end, we apply the Gaussian phase-space representation for fermions to dynamical simulations of large scale systems. Earlier work focussed on simulations in imaginary time, to determine the ground-state properties of many-body systems. By contrast, we focus on the *real-time* dynamics of many-body quantum systems, a class of problems for which few practical exact methods exist.

For the first application of the fermionic phase-space method to a multimode dynamical problem [1], we consider the dissociation into pairs of correlated fermionic atoms of a uniform 1D molecular BEC initially in a coherent state at zero temperature. Assuming sufficiently low densities, we neglect s-wave scattering interactions to simplify the treatment. We simulate systems with $M = 10^3$ relevant atomic Fourier modes and $N_0 = 10^2 - 10^4$ ($^{40}K_2$) molecules at densities $n_{1D} \simeq 1.3 \times 10^5 - 1.3 \times 10^7$ m^{-1}. In these cases, the number-state calculation is impossible as the dimension of the Hilbert space is enormous ($d = 2^M n_{\max} \gg 10^{300}$). In regimes where there is large molecular depletion, we see the growth of strong correlations, in contradiction to the approximate mean-field results. We were able to benchmark a semiclassical approach, with number-uncertainty built into the initial conditions, that qualitatively reproduces the large $g^{(2)}_{\rm mm}$ correlations seen in the molecular field (Fig. 1b).

Although we report here only on 1D simulations, we have also implemented 2D and 3D calculations and found that the method works reliably in higher dimensions. We have also explored how different mappings to stochastic equations can dramatically alter the performance of the numerical simulations [2].

In work in progress, the Hubbard model of interacting fermions on a lattice has been implemented and, for small lattices, is being checked against exact number-state calculations. As well as the intrinsic interest of the Hubbard model, this work will allow fermionic models with s-wave scattering to be simulated exactly. It also provides a convenient starting point for introducing a range of efficient approximate approaches that can then be benchmarked.

References

[1] M. Ögren, K. V. Kheruntsyan, and J. F. Corney, Europhysics Letters **92**, 36003 (2010).
[2] M. Ögren, K. V. Kheruntsyan, and J. F. Corney, arXiv:1008.0970v1, Computer Physics Communications , in press (2011).