Exact Quantum Dynamics of Fermionic systems

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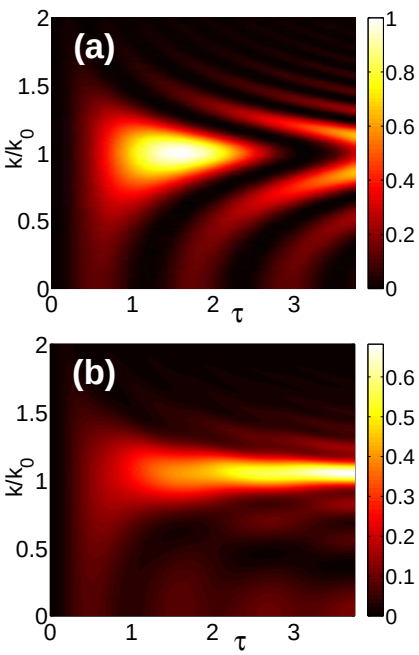
The physics of interacting fermions is the basis of many of the most important phenomena in condensed matter physics, ultracold gases, and quantum chemistry. A fundamental issue is how the microscopic interactions at the quantum level give rise to collective and emergent effects in many-body systems. 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 and to validate the potential simulators, or to benchmark approximate approaches, a numerical simulation of the exact real-time dynamics is required.

To this end, we are adapting the Gaussian phase-space representation for fermions to dynamical simulations of large scale systems. This representation was used to give a sign-free simulation method for determining the ground-state properties of the Hubbard model, thereby giving insight into the origin of high-T_c superconductivity in cuprates [1]. By contrast, we are focussing on the *real-time* dynamics of many-body quantum systems, a class of problems for which few practical exact methods exist.



Time-evolution of atomic momentum densities in (a) Pauli-blocked and (b) depleted regimes.

For the first application of the fermionic phase-space method to a multimode dynamical problem [2], we consider the dissociation into pairs of correlated fermionic atoms of a uniform molecular BEC (MBEC) initially in a coherent state at zero temperature. Assuming sufficiently low densities, we neglect s-wave scattering interactions to simplify the treatment. We simulated 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 ($d = 2^M n_{\max} \gg 10^{300}$). We find different regimes of dynamical behaviour: (a) if the initial number ($N_0 = 10^4$) is much larger than the number of available atomic modes, the dynamics is dominated by Pauli blocking and is well-described by a pairing mean-field theory; (b) if the number of molecules is comparable (or less) than the number of available modes, we see large molecular depletion and the development of strong correlations. In this regime, the atom pairs develop beyond-mean-field correlations, in addition to becoming correlated with the molecular field, leading to large fluctuations in the second-order correlation function of the molecules.

Although we have here reported only on 1D simulations, we have also implemented 2D and 3D calculations and found that the method works reliably in higher dimensions. Extensions of the method to implement s-wave scattering interactions will enable the study of non-equilibrium dynamics in a broader class of fermionic systems of current experimental interest, such as atomic Mott insulators in optical lattices and the BCS-BEC crossover problem.

References

[1] T. Hardy, J. Hague, J. Samson, A. Alexandrov, Phys. Rev. B **79**, 212501 (2009).
[2] M. Ögren, K. V. Kheruntsyan and J. F. Corney, arXiv:0910.4440, *Submitted to Phys. Rev. Lett.* (2009).