Fermionic phase space method for exact quantum dynamics

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Numerical approaches are an indispensable part of endeavours to understand quantum many-body physics in condensed matter and AMO physics. In particular, there is a need for real-time, dynamical simulations, driven in large part by the progress in the control and flexibility of ultracold atom experiments, which has made the dynamically evolving quantum many-body state directly accessible. For bosons, first-principles phase-space methods have successfully simulated dynamics in experimentally realistic systems [1]. However, these methods are not directly applicable to fermionic systems, which are an increasingly important area of ultracold atoms, often with direct relevance to condensed matter systems.

In this work we employ a Gaussian stochastic method based on a generalized phase-space representation of the quantum density operator [2]. We use the method to calculate the dynamics of the production of correlated pairs of fermionic atoms by dissociation of a Bose-Einstein condensate (BEC) of diatomic molecules [3]. This work represents the first application of this fermionic phase-space method to the dynamics of a multimode system of many interacting particles.

The Gaussian phase-space method provides an exact solution to quantum dynamics, as long as sampling error can be controlled. It can be viewed as providing the quantum corrections, through additional stochastic terms, to different mean-field approaches.

The simulations take a uniform molecular BEC (MBEC) in a coherent state as the initial condition. Assuming sufficiently low densities, we neglect s-wave scattering interactions. The Hamiltonian is then given by

$$\widehat{H} = \hbar \sum_{\mathbf{k},\sigma} \Delta_{\mathbf{k}} \hat{n}_{\mathbf{k},\sigma} - i\hbar\kappa \sum_{\mathbf{k}} \left(\hat{a}^{\dagger} \hat{m}_{\mathbf{k}} - \hat{m}_{\mathbf{k}}^{\dagger} \hat{a} \right), \tag{1}$$

where $\mathbf{k}$ labels the plane-wave modes and $\sigma = 1, 2$ labels the effective spin state for the atoms. The fermionic number and pair operators are defined as $\hat{n}_{\mathbf{k},\sigma} = \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma}$ and $\hat{m}_{\mathbf{k}} = \hat{c}_{\mathbf{k},1}\hat{c}_{-\mathbf{k},2}$, respectively, with $\{\hat{c}_{\mathbf{k},\sigma}, \hat{c}^{\dagger}_{\mathbf{k}',\sigma'}\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$, while the bosonic molecular operators obey $[\hat{a}, \hat{a}^{\dagger}] = 1$.

The essence of the phase-space approach is the mapping of the density operator evolution into a Fokker-Planck equation for a phase-space distribution, in this case via a continuous Gaussian operator basis [2]. The evolving distribution is then sampled with stochastic differential equations (SDEs) for the phase-space variables that are structurally similar to the Heisenberg equations for the corresponding operators. The stochastic equations are far from being unique and can be tailored (e.g., by the choice of diffusion gauge [4]) to give SDEs with different numerical properties.

Our 1D simulations involved $M = 10^3$ atomic modes and $N_0 = 10^2 - 10^4$ ($^{40}K_2$) molecules. In these cases, the number-state calculation is impossible as the dimension of the Hilbert space is enormous ($d = 2^M n_{\max} \gg 10^{300}$). The results reveal significant higher-order correlations that cannot be accounted for by the approximate pairing mean-field theory. We have also performed 2D and 3D simulations with the method.

Despite the intrinsically greater complexity of fermionic systems, the Gaussian phase-space method brings us to the situation similar to what one finds in purely bosonic systems by going from the simplest mean-field description to more exact treatments to understand quantum correlations. Extensions of this method to implement s-wave scattering interactions will allow us to study non-equilibrium dynamics in a broader class of fermionic model systems of current experimental interest, such as the Fermi Hubbard model and the BEC-BSC crossover problem.

References

[1] P. Deuar and P. D. Drummond, Phys. Rev. Lett. **98**, 120402 (2007); A. Perrin *et al.*, New J. Physics **10**, 045021 (2008); C. M. Savage, P. E. Schwenn and K. V. Kheruntsyan, Phys. Rev. A **74**, 033620 (2006).

[2] J. F. Corney and P. D. Drummond, Phys. Rev. Lett. **93**, 260401 (2004); Phys. Rev. B **73**, 125112 (2006); J. Phys. A: Math. Gen. **39**, 269 (2006).

[3] M. W. Jack and H. Pu, Phys. Rev. A **72**, 063625 (2005); K. V. Kheruntsyan, Phys. Rev. Lett. **96**, 110401 (2006).

[4] C. W. Gardiner, *Handbook of Stochastic Methods*, Springer, 3rd ed. (Springer, Berlin, 2004).