Correlated quantum dynamics with fermionic TWA

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Problem

We investigate a new fast method for modeling time evolution of electrons in correlated materials. All existing methods have draw-backs, Exact Diagonalisation scales exponentially with the systems size, Mean-Field methods do not model correlation and Density Matrix Renormalisation Group are usable only in 1D.

We present here the dynamic simulation of a Fermi-Hubbard system computed with fermionic Truncated Wigner Approximation (fTWA). fTWA scales quadratically with the systems size and take into account electron correlation, this is a promising method for modeling large, 2D and 3D, correlated systems.

Fermi-Hubbard Model

We use a Fermi-Hubbard Hamiltonian :

$$\hat{H} = -\sum_{i,j,\sigma} j_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i,j} u_{ij}\hat{c}^{\dagger}_{i\uparrow}\hat{c}^{\dagger}_{j\downarrow}\hat{c}_{i\uparrow}\hat{c}_{j\downarrow}, \tag{1}$$

- j_{ij} is the hopping interaction of p_z orbitals between sites i and j.
- u_{ij} is the interaction between two particles of opposite spins on sites i and j.

We only consider equal hopping between neighbour sites: $j_{ij} = J$ if i and j are neighbours, we also limit to systems with on-site interactions: $u_{ij} = U$ if $i = j$.

Phase-Space Method

Fermionic Truncated Wigner Approximation (fTWA) belongs to the Phase-Space representation methods in which we formulate our problem via an expansion of the density operator $\hat{\rho}$ over an over-complete operator basis $\hat{\Lambda}(\boldsymbol{\lambda})$ indexed by the phase-space variables $\boldsymbol{\lambda}$:

$$\hat{\rho} = \int P(\boldsymbol{\lambda})\hat{\Lambda}(\boldsymbol{\lambda})d\boldsymbol{\lambda}\,. \tag{2}$$

The time evolution of the density $P(\boldsymbol{\lambda})$ is governed by a PDE for P, and the observable values $\langle\hat{\mathcal{O}}\rangle$ are recovered using averages of P with corresponding weight functions $\mathcal{O}_P(\boldsymbol{\lambda})$ [1].

Fermionic Truncated Wigner Approximation

Symmetry properties of the chosen operators $\hat{\Lambda}(\boldsymbol{\lambda})$ in the Wigner-Weyl formalism, cause even-order terms in the PDE of $P(\boldsymbol{\lambda})$ to disappear. Truncating the PDE after 2.nd order derivatives, we then have a first-order PDE:

$$\frac{\partial}{\partial t}P(\boldsymbol{\lambda},t) = \frac{\partial}{\partial\boldsymbol{\lambda}}A(\boldsymbol{\lambda})P(\boldsymbol{\lambda},t)\,. \tag{3}$$

On a practical point of view, we compute multiple trajectories with initial conditions drawn from the initial density $P(\boldsymbol{\lambda},0)$. Those trajectories represent the evolution of the density, and observables are recovered by computing its averages and covariances[2].

Results

We apply our method on hexagonal lattices, in this example a 10-sites system made of two hexagones, see figure 1. In figures 2, 3, 4 and 5, the dashed black line is the Exact Diagonalisation solution, the dash-dotted red one is computed with the mean field method and the blue one the fTWA method. We first plot site occupations, both for short-time dynamic (figure 2) and for long-time dynamic (figure 3) to see the improvements of the fTWA method over the mean-field method.

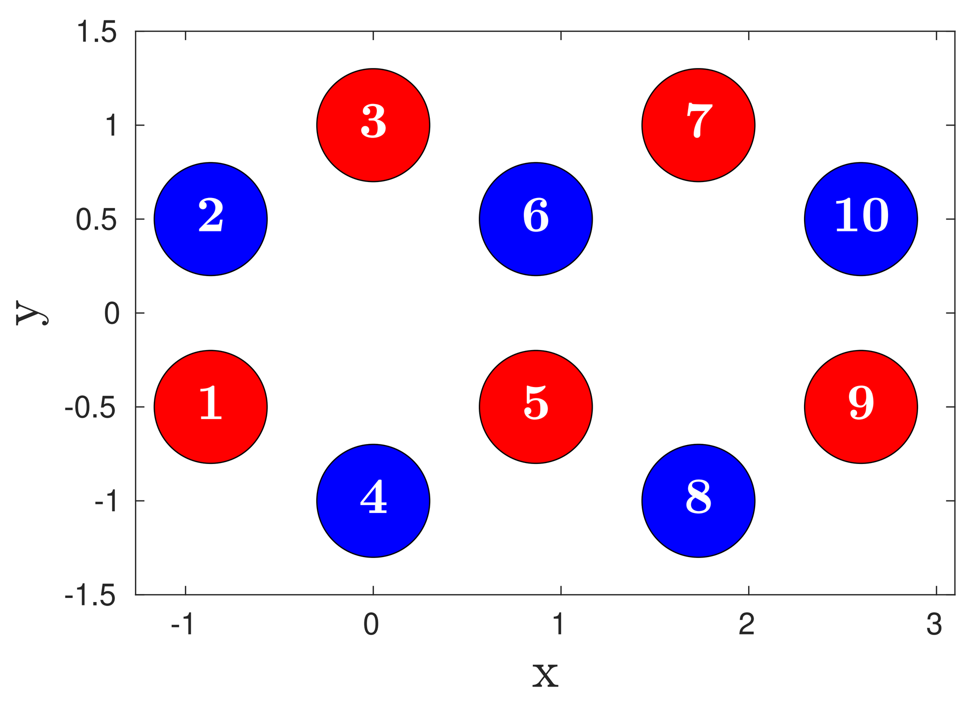

Figure 1: Geometry of the 10-sites system, in red sites with up-spin electrons, in blue site with down spin particles.

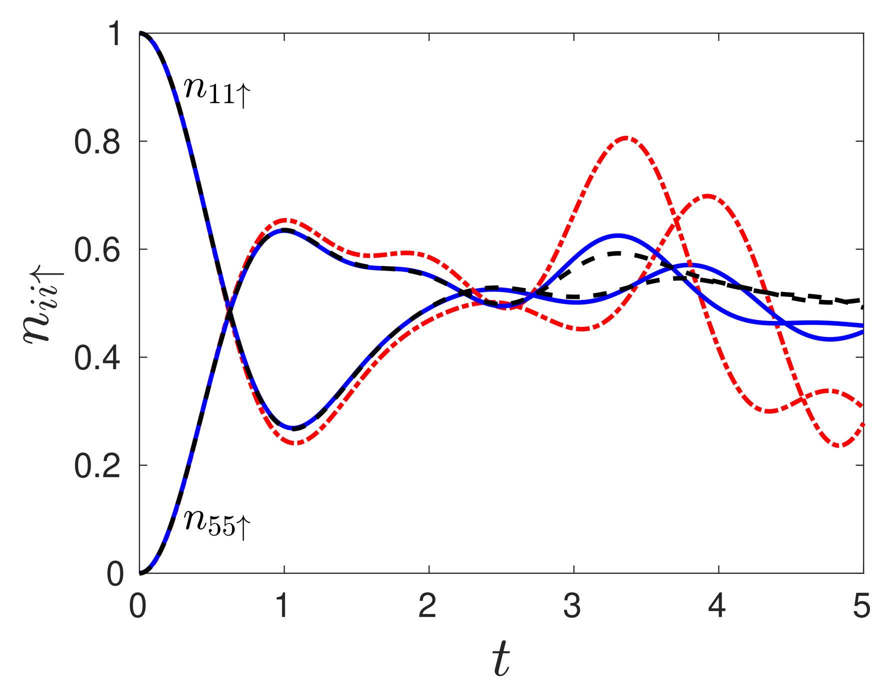

Figure 2: Site occupation of up-spin electron in sites 1 and 5. The mean-field method is exact until $t \simeq 1$ and fTWA until $t \simeq 3$.

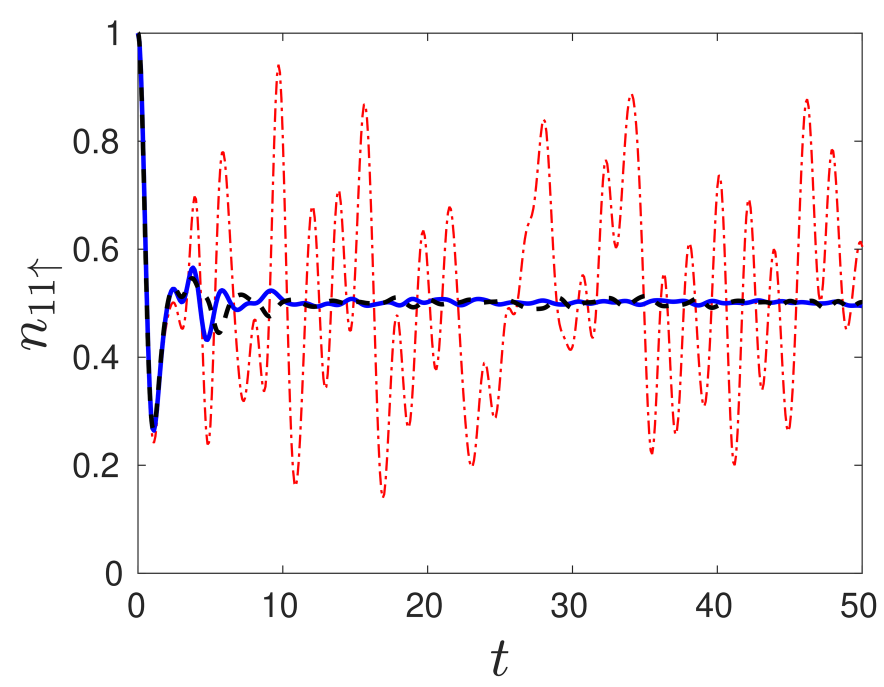

Figure 3: Site occupation of up-spin electron in sites 1 for a longer time. fTWA also model the damping of long-time dynamics.

We then plot sites correlations between spaced sites (figures 4), neighbour sites (figure 5), we see that contrary to the mean-field method, fTWA is able to reproduce short-time site correlation. In figure 6, we plot the site correlation for different system sizes (4, 6, 10 and 198 sites), fTWA can also model correlation in stabilized systems.

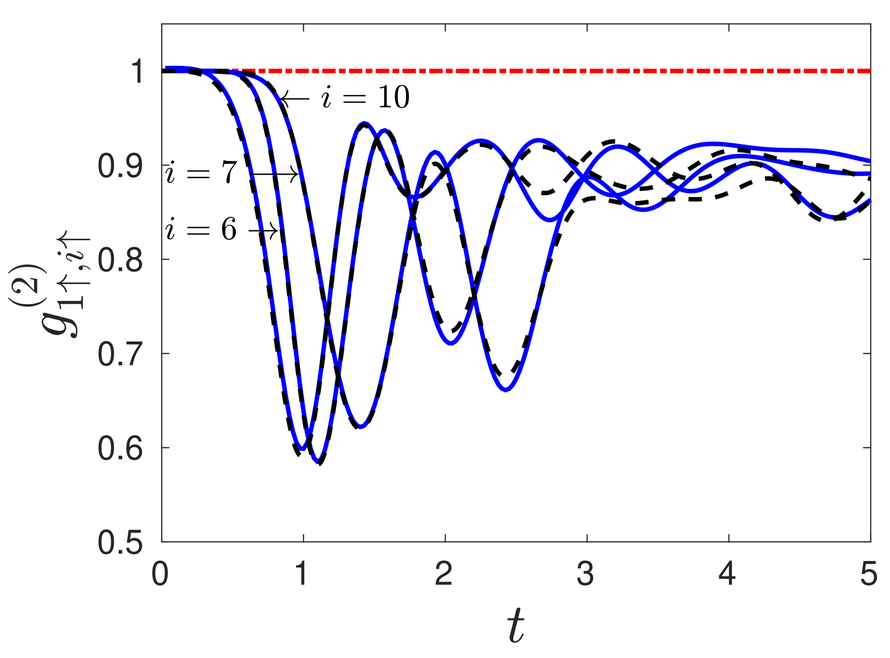

Figure 4: Correlation function $g^{(2)}_{1\uparrow,i\uparrow}$ between up-spin particle on site 1 and up-spin particle on site 6, 7 and 10.

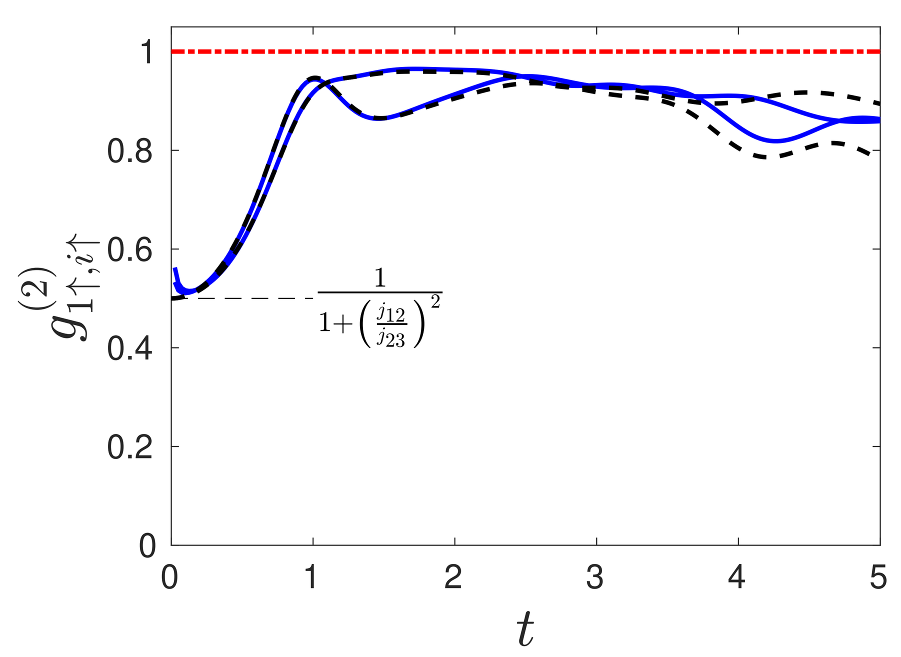

Figure 5: Correlation function $g^{(2)}_{1\uparrow,i\uparrow}$ between up-spin particle on site 1 and up-spin particle on site 6, 7 and 10. The short-term limit ($t \simeq 0$) is well modeled, here $g^{(2)}_{1\uparrow,2\uparrow} = 0.5$.

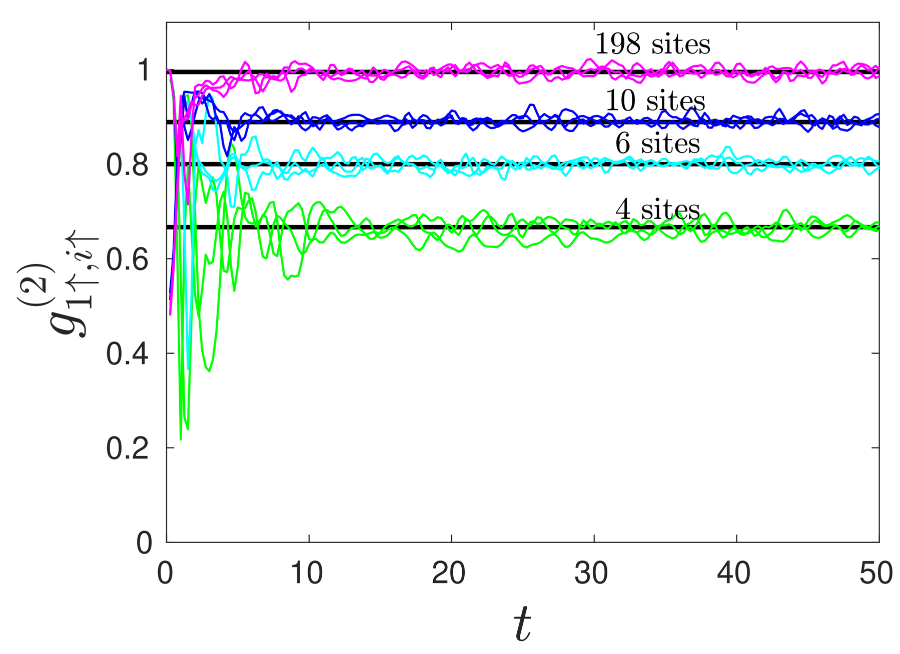

Figure 6: Correlation function $g^{(2)}_{1\uparrow,i\uparrow}$ between up-spin particle on site 1 and up-spin particle on site 2, 3 and 4 for different system size. fTWA is able to model the average of these correlations even for large times.

[1] Adam S Sajna and Anatoli Polkovnikov. “Semiclassical dynamics of a disordered two-dimensional Hubbard model with long-range interactions”. In: *Physical Review A* 102.3 (2020), p. 033338.
[2] F Rousse, O Eriksson, and M Ögren. “Correlated quantum dynamics of graphene”. In: progress 2022.