**Introduction**

Cold atoms in optical lattices: can artificially create multitude of systems strongly/weakly correlated, attractive/repulsive interactions. Can be tuned to be described by the Hubbard model, a lattice model with on-site interactions.

**Question:** How does repulsive interactions change the dynamical behavior of fermions?

We will study how fermions, initially trapped in a parabolic trapping potential, move when we remove the confine. To this end, we use Time Dependent Density Functional Theory (TDDFT) originating from the Runge-Gross theorem [1].

Why TDDFT for cold atoms?

- Variety method, applicable to a wide of systems
- Computationally cheap propagation of single-particle equations

(Kohn-Sham equations) moving in an effective local potential.

Local potential treats interactions as $\tilde{v}_{ij}+\tilde{v}_{ij}$ Hartree potential + the exchange-correlation potential, universal potential

Trouble: TDDFT for strongly correlated lattice models hard using the usual weakly correlated systems the electron gas.

Verdesi (2008) [2]; TDDFT possible in 1D. Accurate densities can be obtained by using a ground state $\rho_0$ coming from a strongly correlated reference system [3] in the adiabatic local density approximation (ALDA), where $\rho_0$ local in space and time, $\rho_0(t) = \rho_0(\tilde{r}(t))$.

**Model**

The model used is the 1D Hubbard model

$$ R = -\sum_{\langle i,j \rangle \in \mathcal{N},\omega_n} t_{ij} c_{j\omega}^\dagger c_{i\omega} + \sum_{\omega_n} \varepsilon_i n_i + V(\tilde{r}) $$

where $\tilde{v}_{ij} = \mathbf{U} n_i^2 n_j$ and $\varepsilon_i = \frac{1}{2} \mathbf{U}^2$. 

To obtain the ground state density, we solve the single-particle Kohn-Sham equations self-consistently:

$$ \tilde{T} + \tilde{v} \rho = \varepsilon \rho; $$

To time evolve, we propagate the time-dependent Kohn-Sham orbitals using a predictor-corrector split-operator method.

$$ \tilde{T} + \tilde{v}(\tilde{r}(t)) \rho(t) = i\hbar \dot{\rho}(t) $$

The single particle density is obtained from $\rho_i = \sum_n | \psi_i(\omega)|^2$

**Results**

- **Ground state:** Density and entanglement entropy for the ring
- Different colors correspond to different sites in the time evolution figures below. The ground state has several phases: (V) Vacuurn, (L) Luttinger liquid, (M) Mott insulator half-filling and (D) Band insulating phase. 'Mott plateaus' due to fermions-fermions interactions; higher interaction gives wider plateaus.
- **Time evolution results:** Density, Entropy

**Local gap**

- To further understand the resistance to change for the Mott insulator, we introduce a new quantity: the local gap, defined as $E_{\text{local}} = E(N+1) - E(N+1) - 2E_g(N)$ where $E(N+1)$ is the expectation value of the Hamiltonian, when we have added (removed) one particle at a specific site. A numerically convenient formula can be derived:

$$ E_{\text{local}} = E(N+1) - E(N+1) - 2E_g(N) $$

- Local gap as a function of time, for the adiabatic perturbation.
- Local gap is always higher for a Mott phase than for a metallic phase.

**Conclusions**

In summary, our study show that:

- The time evolution of the expanding cloud displays a wide variety of non-equilibrium phenomena (overshooting, transients, self-induced stability, etc.) all of which should be experimentally accessible with todays technology.

In particular, optical experiments can be used to investigate the time evolution of the Mott insulator - a state of matter that in ordinary condensed-matter situations can only be studied in static situations;

- The connection between the entanglement entropy and changes of phase extends from equilibrium to non-equilibrium situations, which opens a wide field for investigations and applications of quantum information concepts in dynamical settings.

- If accurate enough potentials are used, TDDFT is a useful tool for characterizing and analyzing the long-time behavior of the expanding cloud, allowing one to describe phenomena such as the approach to the ground state, and thermalization of initial states that are far from equilibrium.

For a more details, please see the article [3].

**References**