Ultra-cold Hubbard fermions in optical lattices

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We present new results for interacting quantum Fermi gases, confined in an optical lattice. Finite temperature atomic correlations are calculated using a novel Gaussian representation. Luttinger liquid theory and the local density approximation let us calculate collective mode frequencies at the metal-insulator transition.

Confining ultracold fermions in an optical lattice presents an outstanding opportunity for implementing the famous Hubbard model. New theoretical techniques are also essential. Here, we present a novel and exact Gaussian phase-space method for fermion systems, which is used to calculate finite temperature atomic correlations. Unlike traditional QMC, there is no resulting Fermi sign problem. Transport properties are also of much fundamental significance. Luttinger liquid theory and the local density approximation let us calculate collective mode frequencies at the metal-insulator transition, giving a strong frequency dip at the onset of the metal-insulator transition as a ‘smoking gun’ to indicate the presence of Mott insulator behavior.

We first address the issue of how to carry out exact numerical calculations in fermionic many-body physics. Recent pioneering experiments in strongly-interacting ultra-cold Fermi gases have opened many experimental regimes in which such physics can be investigated with unprecedented simplicity and precision, both in the BEC-BCS cross-over regime, and in lattices. The underlying atomic interactions are extremely well-understood, and the dynamics, interactions and geometry are all highly adaptable. Measurement techniques are also rapidly improving, with direct measurements of momentum correlations being recently reported. This situation provides a substantial opportunity to develop and test novel first-principles theoretical methods for the investigation of correlations and dynamical effects in these novel quantum systems.

To this end, we introduce a general Gaussian operator basis for fermionic density operators. Like the analogous basis for bosons, the Gaussian basis enables a generalised phase-space representation of arbitrary physical density operators as a distribution over the phase-space. We prove three central results: the basis is complete, the distribution can always be chosen positive, and there are mappings to a second-order differential form for all operator products up to quartic order. Hence, positive-definite Fokker-Planck equations exist for many-body fermionic systems. This leads to first-principles stochastic simulation methods, either in real time or at finite temperature.

The Gaussian phase-space representation therefore gives a solution to a long-standing problem in theoretical physics, which is the sign problem that occurs in many-body fermionic wavefunctions. The ideal system to demonstrate these strong fermionic correlations, and to test our predictions, is the Hubbard model of fermions in a lattice, which is now able to be implemented directly using optical lattices.

The results are different for fermions and for bosons, since because of the Pauli exclusion principle, at least two distinct spin eigenstates are needed to have on-site interactions with fermions. This leads to the (fermionic) Hubbard model,

\[
\mathcal{H} = - \sum_{j,\sigma=\pm 1} t_{ij} \left( \hat{a}_{i,\sigma}^\dagger \hat{a}_{j,\sigma} + h.c. \right) + U \sum_{j} \hat{n}_{j,+} \hat{n}_{j,-} + \sum_{j,\sigma=\pm 1} V_j \hat{n}_{j,\sigma},
\]

where \( V_j \) includes the external trap potential which we assume is harmonic, \( U \) gives rise to on-site interactions, and \( t_{ij} \) describes tunneling between the sites. This model of interacting fermions
is also used in high-$T_c$ superconductivity, where it is more qualitative than quantitative in its applicability. The dimensionality and lattice structure of the model determine the tunneling matrix $t_{ij}$.

In a single-band model as given above, one can expect a band insulator to form in the non-interacting limit, when all available sites have been occupied (i.e., two particles per site). However, this is complicated by the existence of the external potential. For a large, deep trap, the density increases towards the centre, so that the insulating region becomes localised, coexisting with a conducting region in the wings.

When there are strong repulsive on-site interactions, the system develops a new band structure in which an insulating region forms at half-filling, i.e., with only one particle per site, as illustrated in the figure.

In order to describe the collective modes, we can make use of the Luttinger long-wavelength Hamiltonian, valid for small displacements. Because of the spin-density separation in the Hamiltonian, there are two types of waves present, described by the indices $\nu = \rho, \sigma$. Using the local-density approximation together with known exact results in one dimension, we can therefore solve the resulting wave-equations for the collective mode frequency, with zero-current boundary conditions at the boundaries where the density vanishes.

The results show a sharp frequency dip as an unmistakable signature of Mott metal-insulator transition (MMIT) physics. This occurs just at the filling factor where the insulating region starts to form at the trap centre.

However, there are some limitations to these methods. In particular, this is a linearized method, and hence is only valid for small displacements; it also only applies to zero temperature.

Preliminary results in the non-interacting case using the Boltzmann equations show that there are additional damping effects that are proportional to displacement. This leaves an unsolved problem, of how to deal with finite temperatures and large displacements in the interacting case.

Nevertheless, the physical effect involved is simple to understand. Collective modes involve large density currents, which propagate through the lattice with a characteristic velocity $u_\nu$. These velocities tend to zero in the neighborhood of an insulating region, and must be exactly zero inside the insulator. This effect slows down transport processes and therefore reduces all collective mode frequencies, which scale as $velocity/length$. The effect is strongest just when the insulating region starts to form, leading to a large fraction of the conducting region having a low average velocity. As the insulating region grows, the part of the trap that is conducting is localized to the wings, so the frequency increases again due to the smaller characteristic lengths involved.