Simulating correlated fermions

We explore the fantastic world of correlated fermions using various simulation tools, including the (time-dependent) density functional theory, quantum Monte Carlo approach and the dynamical cluster approximation. These simulation methods allow us to answer many key questions related to experiments on the ultracold Fermi gases and correlated topological insulators.

1 Simulating strongly correlated fermionic atomic gases

1) Thermodynamics and magnetic properties of Fermi gases in optical lattice

Reaching the antiferromagnetic Néel state is the next important milestone in experiments on ultracold fermionic gases. Below the Néel temperature one will enter the regime where intriguing physics (e.g. d-wave superconductors) due to strong correlations may appear.

Motivated by a recent experiment in the Esslinger's lab in ETH [1], we study the 3D Hubbard model with anisotropies in the tunneling amplitudes [2]. In agreement with the experiment, we find that the nearest neighbor spin correlations are significantly enhanced in the direction with stronger tunneling. Furthermore, using our results as a thermometer we show that the experiment has reached a temperature comparable to the strong tunneling amplitude. However, since the Néel temperature drops with the anisotropy it is not advised to pursue the magnetic long range order in the anisotropic systems.

Ultracold fermions with multiple spin components [3,4] are also of great interest because there is no counterpart in the condensed matter systems. The large number of spin components enhances quantum fluctuations and may lead to exotic quantum states. Along this line we have investigated the thermodynamics of half-filled SU(N) Hubbard model on square lattice and found the spin-fluctuation facilitates the Pomeranchuk cooling for the SU(6) case [5]. We also investigated the ground state magnetic properties of SU(N) Hubbard model [6] and found reduced or even vanishing magnetic moments.

2) Itinerant Ferromagnetism in ultracold fermions

Previous experimental effort of stabilizing of the itinerant ferromagnetism state in ultracold fermions was hindered by the metastable nature of the gas at large positive scattering length [7,8]. We employed the previously developed density functional theory for ultracold fermi gases [9] to investigate the problem [10] and suggested to impose a shallow optical lattice to stabilize the ferromagnetic phase. Because of reducing kinetic energy in an optical lattice the ferromagnetic phase extends to smaller scattering lengths, which alleviate the stability issue and make experimental observation possible.

2 Band topology and dynamics of fermonic atomic gases

Recent technical advances have allowed experimentalists to build complex optical lattices with nontrivial band structures. We have pointed out several directions to explore interesting topological and dynamical behaviors in these new generation "beyond standard" optical lattices.

1) Topological charge pumping and Hofstadter butterfly

We proposed an experiment setup to realize the long sought topological charge pumping [11] in a one-dimensional optical lattice [12]. It provides a way to accurately control the atom flow and is a dynamic analog of the integer quantum Hall effect. The topological pumping also suggests a general way to measure topological invariants of two dimensional optical lattices. We proposed a hybrid time-of-flight experiment [13] to directly measure, for example, the Chern number of the Hofstadter lattice realized in the Munich and MIT group recently [14,15]. We devised a method to observe the so called Hofstadter butterfly [16]- a beautiful fractal energy spectrum- by formulating it as a deconvolution problem and suggested an algorithm to solve it even with experimental noises [17].

2) Bloch oscillation and Berry phases

Collaborating with Esslinger's lab in ETH, we studied Bloch oscillations of Fermi gas in a tunable honeycomb optical lattice. Our numerical simulations explained the observed interband transition fraction [18,19]. Furthermore, we predicted real-space drifts due to the Berry phase effect at the Dirac point, which can be used to verify future experimental setups with nontrivial band structures.

3 Topological insulators with strong interaction

A topological insulator is a material behaviors like an insulator in its interior but whose surface contains conduction states, which is stable against symmetry preserving perturbations. Topological insulators have caught much attention in the condensed matter physics in recent years, yet most studies are based on noninteracting Bloch bands. There are, in general, two difficulties when studying interacting effect in topological insulators: the lack of unbiased numerical methods and the difficulty of direct quantification of the topological property of an interacting system.

We have shown it is possible to extract topological indices from interacting Green's functions [20,21]. Combined with the dynamical-mean-field theory and the unbiased quantum Monte Carlo simulations, this allows us to characterize the interaction induced topological phase transitions in two prominent models for topological insulator: the Bernevig-Hughes-Zhang model [22] and the Kane-Mele model [23,24]. We also applied the topological pumping idea to the Hofstadter-Hubbard model [25] and observed a sharp topological signature at the phase transition from a quantum spin Hall to a superfluidity state.

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