Application of low-energy theories to describe the dynamics of doublons in the Bose-Hubbard model on a honeycomb lattice

Holger Niehus[1] **and Daniela Pfannkuche**[1]

[1] *I. Institute for Theoretical Physics, University of Hamburg, Jungiusstr. 9, D-20533 Hamburg, Germany*

Identifying the relevant processes for the dynamics of excitations far from equilibrium is one of the most challenging tasks in many particle physics. We approach this problem for a special class of excited states in the Bose-Hubbard model, so-called doublons, by means of effective low-energy models in conjunction with exact diagonalization.

In 2002 the superfluid to Mott-insulator transition has been observed for an ultra-cold Bose gas in an optical lattice and it was subsequently shown that theses systems can be used to simulate Hubbard models with precise control over the model parameters [1]. Furthermore, low-dimensional systems or unconventional geometries like the honeycomb geometry (best known from graphene) can be realized, the latter was shown recently [2]. With the additional ability to tailor particular initial states, this enables us to study many new effects of the Hubbard model in the absence of dissipation.

We are all familiar with composite objects created by attractive interactions, but in a periodic system and without a channel to dissipate energy, particles may be bound together also by repulsive forces. For the Bose-Hubbard model the existence of a band gap in conjunction with energy conservation prohibits the conversion of the interaction-energy of two particles on the same site – a doublon – to kinetic energy of the particles, rendering the direct decay impossible. This stability of doublons was recently observed experimentally for both ultra-cold bosons and fermions in optical lattices, where long lifetimes were measured in case of large repulsive interactions of the atoms [3, 4].

We use a method called Löwdin downfolding to derive effective low-energy models for the dynamics of doublons in two different environments. This perturbative approach is expected to be accurate in the limit of $t \ll U$. Using exact time evolution for small systems under periodic boundary conditions enables us to validate the quality of our effective models.

First we study the interaction of few doublons by creating two doubly occupied sites in an otherwise empty lattice. Its low-energy theory of third order in the hopping is recast to a doublon-doublon Hamiltonian capturing the essential dynamics. We show that all but second-order terms vanish. One is left with a next-neighbor hopping of the doublons and a strong next-neighbor interaction of the doublons, which prevents neighboring doublons from delocalizing completely. We also show that the application of this model to many doublons is limited and identify the mechanism responsible for it breaking down.

Complementary we study the influence of neighboring bosons on the dynamics of a single doublon in a unit filled lattice. We show that the dynamics of such systems may be described by a doublon-holon model. Here the doublon is no longer increasingly immobile for increasing U, but rather is able to delocalize in first order. Furthermore, we observe that the next-neighbor doublon-holon attraction is particularly weak and unable to bind them together.

[1] M. Greiner et al., Nature **415**, 39 (2002).
[2] P. Soltan-Panahi et al., Nature Physics **7**, 434 (2011).
[3] K. Winkler et al., Nature **441**, 853 (2006).
[4] N. Strohmaier et al., Phys. Rev. Lett. **104**, 080401 (2010).