Two-Dimensional Dynamics of Ultracold Atoms in Optical Lattices

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We analyze the dynamics of ultracold atoms in optical lattices induced by a sudden shift of the underlying harmonic trapping potential. In order to study the effect of strong interactions, dimensionality and lattice topology on transport properties, we consider bosonic atoms with arbitrarily strong repulsive interactions, on a two-dimensional square lattice and a hexagonal lattice. On the square lattice we find insulating behavior for weakly interacting atoms and slow relaxation for strong interactions, even when a Mott plateau is present, which in one dimension blocks the dynamics. On the hexagonal lattice the center of mass relaxes to the new equilibrium for any interaction strength.

The possibility to confine ultracold atoms in optical lattices has opened up a new research area, where interacting quantum many-body systems consisting of bosons \[1\,2\] and fermions \[3\,4\] can be studied with unprecedented high precision and tunability \[2\]. A new and exciting development is to study the dynamics and out-of-equilibrium behavior of those systems, see e.g. \[6\], which can also be used as an experimental probing technique \[5\,8\]. In particular, it is possible to bring the system far out of equilibrium by performing an instantaneous shift in the underlying harmonic trapping potential. In this way particle transport can be investigated. This procedure is schematically illustrated in Fig. 1. Experiments in this setup with a three-dimensional Bose-Einstein condensate subject to a one-dimensional optical lattice revealed a transition from coherent to dissipative behavior \[3\,10\,11\,12\]. For a truly one-dimensional gas, the impact of the optical lattice was found to be even stronger: already for small lattice depths dissipative motion was observed \[13\,14\], which has been theoretically investigated with a variety of methods \[15\,16\,17\,18\,19\,20\]. A three-dimensional fermionic cloud subject to a one-dimensional optical lattice showed strongly suppressed center of mass motion \[21\,22\]. Related theoretical \[23\,24\] and experimental \[25\] work on a Bose gas in a moving optical lattice showed a momentum-dependent breakdown of superfluid motion.

However, both experimental and theoretical research in this direction has up to now \[26\] been restricted to a one-dimensional optical lattice. In this Letter we analyze the behavior of repulsively interacting bosons in two dimensions, where geometrical considerations play a profound role. The influence of the lattice dimensionality is most clearly seen when a Mott plateau is formed. Unlike in one spatial dimension, where this leads to insulating behavior \[16\], we find that in two dimensions there is always relaxation of the center of mass to the new equilibrium position. This behavior even persists in the limit of hard-core bosons. Moreover, in two dimensions, one can choose different lattice geometries, which severely influences the dynamics. Experimentally this is possible by varying the angle between the laser beams which make up the optical lattice. Here we compare the behavior on the square lattice to the hexagonal lattice and find remarkably different behavior. This originates from the single particle dynamics, which on the square lattice can be described in terms of Bloch oscillations. Those are absent on the hexagonal lattice, where the atoms move along the equipotential lines. Therefore, strongly interacting bosons on the hexagonal lattice show a much quicker relaxation of the center of mass than on the square lattice. In order to study bosonic atoms with arbitrarily strong repulsive interactions we apply the Gutzwiller mean-field theory. This includes the limit of infinite interaction strength (hard-core bosons).

For a deep optical lattice and moderate filling, the bosons can be described by the single band Bose-Hubbard Hamiltonian

\[ H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \sum_i \left\{ \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + (V(i, t) - \mu) \hat{n}_i \right\} , \]

where \( b_i \) is the bosonic annihilation operator at site \( i \), \( \mu \) is the chemical potential, \( J \) is the hopping amplitude and \( U \) is the on-site repulsion. \( J \) and \( U \) can be expressed in terms of the atomic interparticle scattering length \( a \), mass \( m \) and laser wavelength and intensity \[3\]. We will
use them as effective parameters. $V(i, t)$ is the underlying harmonic potential which we take equal to:

$$V(i, t) = V_0 |x_i - x_0(t)|^2.$$  \hfill (1)

In the following we set $J = 1$ and use $U = U/J$, $\mu = \mu/J$ and $V_0 = V_0/J$ as dimensionless parameters. Time is expressed in units of $\hbar/J$. The shift $A$ in the harmonic potential is expressed in terms of the lattice spacing $a$.

For weakly interacting bosons, a Bose-Einstein condensate forms, whose dynamics can be described by the Gross-Pitaevskii equation. A complementary approach, which is also valid for strongly interacting bosons, is the time-dependent Gutzwiller technique [27] where the coupling between the lattice sites is treated in a mean-field approximation. For inhomogeneous systems, this procedure has to be carried out in a space-resolved version, where with each site a separate order parameter is associated. The total many-body wavefunction is within this approximation given as $|\Psi\rangle = \prod_i \sum_n \Phi_i \Phi_j f_{n+1}^* f_n + \sum_n \sqrt{n} \Phi_j f_{n+1}^* f_n + \sum_n \sqrt{n} \Phi_j f_{n+1}^* f_n - \sum_n \sqrt{n} \Phi_j f_{n+1}^* f_n$.

In practice, the infinite sum over the particle numbers $n$ is replaced by a finite sum, by introducing a cut-off $N_c$ depending on the strength of the interaction and the local density. The dynamics is governed by the set of coupled differential equations [27]

$$i \frac{\partial}{\partial t} f_n^j = - \sum_{i(i)} (\frac{U}{2} n(n-1) + V(i, t) - \mu) f_n^i,$$

where $\Phi_i = \langle b_i \rangle = \sum_n \sqrt{n} (f_{n+1}^i)^* f_n^i$. This Gutzwiller approximation is a highly efficient method for studying dynamics in higher dimensional lattices. It conserves energy exactly and particle number with a very good accuracy. The latter, however, is only true if the sites are sequentially updated: a parallel update of all sites together violates particle number conservation. The validity of the Gutzwiller approximation is further justified by the fact that for small interactions it incorporates the Gross-Pitaevskii dynamics [27]. Also the limit of strong interactions in one dimension is correctly reproduced by the Gutzwiller approximation (see Fig. 3): in that case the dynamics of the center of mass is completely blocked [10]. The Gutzwiller approximation is naturally restricted to zero temperature, since it neglects phase fluctuations. We therefore only consider $T = 0$ here.

We first investigate the influence of the lattice topology on the single particle dynamics, which will reflect itself in the behavior of weakly interacting bosons. For small shifts, the bosons perform dipole oscillations around the shifted center. Interactions between the bosons lead to damping that increases with the strength of the interaction. This behavior is limited to small shifts, for which the shifted wavefunction still has an overlap with the ground-state-wavefunction in the shifted potential. Alternatively, one can argue that for larger shifts the potential energy introduced into the system by performing the shift cannot totally be converted into kinetic energy, which is restricted because of the single-band description. For larger shifts the lattice structure becomes very important, which is most clearly seen in the limit of non-interacting bosons (see Fig. 2). If $U = 0$, the Hamiltonian on the square lattice is the sum of two commuting one-dimensional Hamiltonians, $\mathcal{H}_{x=0} = \mathcal{H}_x + \mathcal{H}_y$ with $[\mathcal{H}_x, \mathcal{H}_y] = 0$. This implies that the dynamics is effectively one-dimensional and the single particle eigenstates are products of the one-dimensional eigenstates, which are highly localized [29]. As a result, the atoms perform Bloch oscillations around the shifted position instead of dipole oscillations after a large shift [30] as shown in Fig. 2b). Because of the non-linearity of the harmonic potential, the Bloch oscillations contain multiple frequencies. Because the eigenstates are localized, the wavepacket remains localized as well (Fig. 2f). The Bloch oscillations persist for small interactions between the bosons, which however cause the Bloch oscillations to be damped, due to dephasing [28]. For stronger interactions the Bloch oscillations disappear. Instead, the center of mass shows dissipative dynamics. This is possible, because in this case the potential energy can be converted into interaction energy, and the center of mass can relax to zero.

The description in terms of Bloch oscillations does not apply to other lattice structures, where the Hamiltonian cannot be decomposed into two commuting one-
dimensional parts. In particular, we have investigated the behavior of free and weakly interacting bosons on a hexagonal lattice. In this case we find for arbitrarily large shifts a relaxation of the center of mass to the minimum of the harmonic potential (Fig. 2a)). Inspection of the density profile shows that this occurs, because on the hexagonal lattice the atoms move along the equipotential lines. The reason for this behavior is, that on the hexagonal lattice plus harmonic potential the single-particle eigenstates form a ring-like structure. Therefore, the bosons perform a ring-like expansion after a large shift and although the center of mass relaxes to the new equilibrium, the atoms actually never do.

It is worth noticing that spinless fermions behave in the same way as weakly interacting bosons. On the square lattice they perform Bloch oscillations after a large shift [22], whereas on the hexagonal lattice the center of mass relaxes to zero, whereas the density forms a ring-like structure. This means that, especially on the square lattice, spinless fermions behave qualitatively different from hard-core bosons. The latter show relaxation of the center of mass to the new equilibrium, as we will demonstrate later. This is unlike the one-dimensional situation, where hard-core bosons behave as free fermions.

We now turn to strongly interacting bosons, for which the dimensionality of the lattice is very important. In one spatial dimension, the motion gets completely blocked when a Mott plateau is present, because the atoms can not pass each other and the center of mass never reaches the new equilibrium position [16]. This behavior is reproduced by our Gutzwiller calculations as shown in Fig. 3. In two dimensions, however, the center of mass motion shows dissipative dynamics and fully relaxes to the new equilibrium (Fig. 4). We did extensive calculations for a wide range of parameters and always found this behavior. The reason is that the superfluid shell can freely move around the Mott-insulating core, thus allowing the system to relax. This is visible in the density plots in Fig. 5 which show that initially the Mott plateau remains inert, but afterwards shows dynamical melting induced by the dynamics of the superfluid ring. Moreover, the insulating plateau scatters the atoms away from their single-particle trajectories, which leads to a significant broadening of the density profile. Therefore, the final state is not the equilibrium state in the shifted potential, because the total energy is conserved. In particular, the Mott plateau has disappeared (Fig. 5). The suppressed density in the center and the broadening of the
density profile is shown in Fig. 6a. We compare this with a finite temperature density profile, which is calculated neglecting phase fluctuations. We derive the temperature from the energy induced in the system by the shift in the potential. This leads to a good agreement, which shows that the density profiles for those parameters thermalize.

The complete relaxation of the center of mass even persists for hard-core bosons. It is worth noticing that the time-scale for the relaxation cannot easily be expressed in terms of the interaction strength, because the relaxation is not due to single-particle tunneling processes. Therefore, the observed relaxation of the center of mass is very slow. This is partly due to the parameters chosen for the simulations; taking a more shallow harmonic potential. This leads to a good agreement, which shows that the density profiles for those parameters thermalize.

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FIG. 6: (Color online) Radial density profile before the shift of the harmonic potential (red) and after relaxation to the new equilibrium (green) for the square lattice (left pictures) and hexagonal lattice (right pictures) for $U = 2$ (upper row) and $U = \infty$ (lower row). The blue line is a thermal density profile. The bosons on the square lattice have relaxed from a shift of six lattice sites; the bosons on the hexagonal lattice relaxed from a shift of ten lattice sites. Other parameters are chosen as $N = 100$ and $V = 0.3$.

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