Creation of a dipolar superfluid in optical lattices

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We show that by loading a Bose-Einstein condensate (BEC) of two different atomic species into an optical lattice, it is possible to achieve a Mott-insulator phase with exactly one atom of each species per lattice site. A subsequent photo-association leads to the formation of one heteronuclear molecule with a large electric dipole moment, at each lattice site. The melting of such dipolar Mott-insulator creates a dipolar superfluid, and eventually a dipolar molecular BEC.

The physics of strongly correlated systems in ultracold trapped quantum gases has attracted a growing interest recently. The experimental progress on the trapping and cooling techniques, and the control of the interatomic potentials by means of Feshbach resonances allow to analyze situations beyond the validity of the mean-field approach. In particular, the possibility to achieve 1D bosonic gases opens the pathways toward a gas of impenetrable bosons [1]. Also, a rapidly rotating trapped bosonic gas should exhibit effects similar to the fractional quantum-Hall effect [2]. The field of strongly correlated atomic systems concerns also ultra-cold Bose gases with large scattering lengths [3,4], and the Mott-insulator (MI) to superfluid (SF) phase transition [5] in gases with large electric dipole moments, which could eventually dominate the physics of the system [6,7].

This Letter is devoted to the analysis of the generation of ultra-cold polar molecules in an optical lattice. We consider the loading of the lattice by a superfluid of two different atomic species, and analyze the transition into a MI phase with exactly one atom of each species per site. This transition is followed by the formation of polar dimers by photo-association, or adiabatic passage. Finally, the quantum melting of the molecular Mott phase into a polar molecular superfluid takes place.

We consider a miscible gas of two trapped atomic bosonic species at very low temperature $T$. Although our calculations could in principle be employed for arbitrary atoms, we have assumed in the calculations below the particular mixture of $^{41}$K and $^{87}$Rb, whose simultaneous Bose-Einstein condensation has been recently realized [2]. We additionally consider that the binary gas is confined in a 2D optical lattice, similarly to the 3D one-component case recently observed in Ref. [8]. The transverse dimension is considered as harmonically confined. The physics of the system is governed by the two-species generalization of the Bose-Hubbard (BH) model, described by the Hamiltonian:

\begin{equation}
H = \sum_{<i,j>}[J_a a_i^\dagger a_j + J_b b_i^\dagger b_j] + U_{ab} \sum_i n_{ai} n_{bi} + \frac{1}{2} \sum_i [U_{0a} n_{ai}(n_{ai} - 1) + U_{0b} n_{bi}(n_{bi} - 1)],
\end{equation}

where $a_i$, $b_i$ are the annihilation operators of $^{41}$K and $^{87}$Rb atoms at the lattice site $i$, which occupy a state described by the Wannier functions $w_{ai}(\mathbf{r} - \mathbf{r}_i)$, $w_{bi}(\mathbf{r} - \mathbf{r}_i)$ of the lowest energy band, localized on this site. This implies that energies involved in the system are small compared to the excitation energies to the second band. We denote the position of the local min-
imum of the optical potential as \( r_i \), and the number operator of K (Rb) atoms at the site \( i \) as \( n_{ai} = \frac{a_i^\dagger a_i}{\sqrt{2}} \). In Eq. (1) only the nearest-neighbor tunneling is considered, which is described by the parameter \( J_{a,b} = \int w_{a,b}(r-r_i) [-\frac{\hbar^2}{2m} \nabla^2 + V_i(r)] w_{a,b}(r-r_j) \, d^3r \), where \( j \) and \( i \) are the indices of neighboring sites, and \( V_i(r) = \sum_{x,y} V_\xi \cos^2(k_\xi x) \) is the optical lattice potential (with wavevector \( k_\xi \)) which we consider to be the same for both species. The optical potential for K and Rb is almost the same for the detunings considered, and to follow the dynamics derived from the time dependent variational principle. The resulting equation becomes:

\[
if_{n,m}^{(i)} = \frac{U_{ab}^2}{2} \sum_{n,m} \langle \Phi_{a}^{n} | a_j | \Psi_{MF} \rangle \Phi_{b}^{m} \sum_{<i,j>} \langle \Psi_{MF} | b_j | \Psi_{MF} \rangle.
\]

When the lattice potential increases, the system follows the changes quasi-adiabatically, and the two species enter sequentially the Mott phase with one atom per site. As shown in Fig. 3 this occurs first for the heavier Rb atoms at \( t \approx 0.75 \) s, and then at \( t \approx 1.5 \) s for K atoms. The ratio \(-U_{ab}/J_a (-U_{ab}/J_b)\) at the transition point equals approximately 23.5 (26), which interestingly compares very well with the expected value, 23.2, for a 2D single-component gas. Therefore the transition point is rather unaffected by the interactions between different species.

At the end of the process each site contains one Rb and one K atom, with a relative atom number fluctuations less than 3%. This, however, requires a sufficient slow modification of the lattice potential, typically within a time scale of 2 seconds for a lattice wavelength \( \lambda = 1064\text{nm} \). Note that the time scale is provided by the inverse of the recoil energy of the lattice, and therefore it scales as \( \lambda^2 \). We note also at this point that a transition 3 times faster leads to about two times larger number fluctuation in the final state. We want to stress that during the whole time evolution the mean number of particles was constant, and equal to the number of lattice sites, which gives us the most complete analogy, within the Gutzwiller approach, to the experimental situation.

Having obtained a Mott phase with one Rb and one K atom per site, a heteronuclear molecule can be generated at each lattice site. One possible mechanism would be two-color Raman photoassociation to make ground state \( ^1\Sigma^+ \) or \( ^3\Sigma^+ \) dimers. Since heteronuclear species do not have gerade/ungerade symmetry, levels of either symmetry could be formed via intermediate excited states of \( \Omega \).
electronic plus spin angular momentum on the molecular axis. Since the Ω states excited at long range typically have mixed singlet and triplet character, photoassociation to ground $[^3\Sigma^+]$ levels is even possible for collision of two doubly spin-polarized atoms, which collide via the ground $[^3\Sigma^+]$ potential. The $1/R^6$ dependence of the excited molecular potential for the case of heteronuclear molecules, in contrast to the $1/R^9$ dependence for the homonuclear case, leads to excitation at relatively short internuclear separation $R$. This difference may lead to reduced Franck-Condon factors for the first excitation step but enhanced factors for the second de-excitation step [24]. In any case, these can be worked out once the potential energy curves of the KRb dimer are better known. A second possible method of making ground state molecules is available for heteronuclear dimers, namely, use of a pulse of microwave radiation to directly associate two colliding atoms in a one-color transition from a scattering state to a bound dimer state. However, the dipole matrix elements within the $[^3\Sigma^+]$ state are small, so this will need fairly high microwave power. Either method will result in an excited vibrational level not far below the dissociation limit. It should be possible to use a succession of Raman pulses to transfer the population from such a level to the ground $v = 0$ vibrational level of the $[^1\Sigma^+]$ or $[^3\Sigma^+]$ state, in a manner similar to that described by Ref. [12]: microwave/infrared pulses may also be feasible for this heteronuclear species. The $[^3\Sigma^+]$ $v = 0$ level has a small dipole moment of 0.0046 atomic units (1 atomic unit is $8.478 \times 10^{-30}$ Cm), whereas it is much larger, 0.30 atomic units, for the $[^1\Sigma^+]$ $v = 0$ level [23]. In the latter case, special care should be taken to prevent the heating due to black-body radiation, which could be avoided by an appropriate shielding.

After the creation of the K-Rb dimers, the system becomes single-component. However, since the molecules have a large dipole moment and are considered to be oriented by an external electric field ($\approx 100$ V/cm), we have to include the dipole-dipole interactions in our calculations. The corresponding Hamiltonian reads [6]:

$$H = J \sum_{<i,j>} b_i^\dagger b_j + \frac{1}{2} U_0 \sum_i n_i (n_i - 1)$$

$$+ \frac{1}{2} U_{\sigma_1} \sum_{<i,j>} n_i n_j + \frac{1}{2} U_{\sigma_2} \sum_{<i,j>} n_i n_j + \ldots,$$

where $b_i$ is the annihilation operator of a heteronuclear molecule at the lattice site $i$. The number operator $n_i$, the Wannier basis $w(r - r_i)$ and the tunneling coefficient $J$ for molecules are defined similarly as in Eq. (6). However, the interaction part significantly differs from that of Eq. (6). The coefficients $U_\sigma$ are defined as follows: $U_\sigma = \int |w(r - r_i)|^2 V_{\text{int}}(r - r_i)|w(r' - r_j)|^2 d^3 r d^3 r'$, where $\sigma = |r_i - r_j|/|k|/4\pi$ is the dimensionless intersite distance. In particular, $U_0$ determines the on-site interactions, $U_{\sigma_1}$ the nearest-neighbor interactions, $U_{\sigma_2}$ the interactions between the next-nearest neighbors, etc. Consequently, the respective summations in Eq. (6) must be carried out over appropriate pairs of sites which are marked by $< \ldots >$ for the nearest neighbors, $<< \ldots >>$ for the next-nearest neighbors, etc. In the 2D calculations presented below, we have taken into account interactions with up to 4 neighbors ($\sigma_1 = 1$, $\sigma_2 = 2$, $\sigma_3 = 2$, $\sigma_4 = 2\sqrt{5}$), since the effects of interactions of a longer range are negligible. In the case of polarized dipoles the interaction potential is

$$V_{\text{int}} = d^2 \frac{1 - 3 \cos^2 \theta}{|r - r'|^3} + \frac{4\pi \hbar^2 a}{M} \delta(r - r'),$$

where the first part of Eq. (4) provides the dipole-dipole interaction characterized by the dipole moment $d$ and the angle $\theta$ between the dipole direction and the vector $r - r'$. The second part of Eq. (4) represents the short-range interactions given by the $s$-wave scattering length $a$ and the molecular mass $M$. We use the dipole moment as 0.3 a.u. [23] and assume the $s$-wave scattering length of K-Rb molecule as $a = \sqrt{\sigma_{\text{KRb}}}$ [5].

FIG. 1. Dynamical transition from the SF phase of $^{41}$K (solid line) and $^{87}$Rb (dashed line) atoms to the MI phase. The upper plot shows the value of the order parameters $\langle |a_i| \rangle$, $\langle |b_i| \rangle$ (constant for all lattice sites) for both species, while the lower one depicts the variance $\text{Var}(n) = \sqrt{(n^2) - \langle n \rangle^2}$ of the on-site occupation. The lattice potential was changed as $V_0(t) = V_{SF} + (V_{MI} - V_{SF})(t/t_0)^3 \exp(1 - (t/t_0)\alpha)$, where $V_{SF} = 4$, $V_{MI} = 19$ in units of recoil energy of $^{41}$K atoms, $t_0 = 1.8$ s for the case of lattice wavelength 1064nm.

We have checked that the MI phase of these heteronuclear molecules is indeed the ground state of the system for a mean lattice filling factor equal to 1. We employ this state as the initial condition for our dynamical calculations of the melting of the Mott phase towards a molecular superfluid. It is, however, interesting to note, that by itself the MI phase of dipolar particles offers promising perspectives as a quantum computation device [20]. The melting dynamics is analyzed by employing again a dynamical Gutzwiller ansatz, but with the Hamiltonian (6). During the dynamics we consider a first stage in which we reduce the lattice trapping potential up to 4 in
recoil energy units of K – Rb molecules. This first stage allows us to reduce the value of $-U_0/J$, but the system remains still in the MI state mostly due to the large contribution of the repulsive dipolar on-site interactions to the $U_0$ coefficient. This process can be performed in a relatively fast time scale compared to the total duration of the melting process, since the MI gap guarantees the adiabaticity at this stage.

Later on, we have observed that the dynamics can be better controlled by modifying the transverse confinement. As shown in Ref. [21], the properties of the dipolar gas strongly depend on the aspect ratio of the on-site wavefunction. In particular, by reducing the transverse confinement, the on-site wavefunction becomes more elongated in transverse direction. As a consequence, $U_0$ decreases, and the system enters into the superfluid phase. Fig. 2 shows this process. Due to the non-completely adiabatic evolution the gas does not exactly follow the expected stationary result, although very clearly a superfluid molecular phase is accomplished. The ratio $-U_0/J \approx 23.2$ at which the transition from MI to superfluid equals surprisingly to the value expected for a 2D single-component gas without a permanent dipole moment. As shown in Fig. 2 this dynamical transition into the superfluid phase occurs for realistic parameters in a time scale of 1s. This transition can be realized, 50 times faster, although the dynamics of the superfluid order parameter is in such case not as smooth as in Fig. 2.

In this Letter we have analyzed the formation of a superfluid of polar molecules. We have considered the loading of a BEC of $^{87}$Rb and $^{41}$K atomic species into an optical lattice. The modification of the lattice potential produces the dynamical transition into a MI phase with only one atom of each species per site. The atoms can then be photo-associated on-site. Once the polar molecules are created, a molecular MI is formed. By reducing the lattice potential and modifying the transverse confinement, such MI evolves into a molecular superfluid within a feasible time scale. Eventually, a molecular BEC is formed. The mechanism studied in this Letter, provides a perspective towards a dipolar BEC.

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24. Also, the on-site densities ($\approx 10^{15}$ cm$^{-3}$) are 1000 times larger than in traditional photoassociation experiments.
25. The value of $a$ is not known, but does not affect our results, since it can always be compensated by transverse confinement, i.e. dipolar forces.