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Creation of a Dipolar Superfluid in Optical Lattices

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We show that, by loading a Bose-Einstein condensate 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 photoassociation leads to the formation of one heteronuclear molecule with a large electric dipole moment, at each lattice site. The melting of such a dipolar Mott insulator creates a dipolar superfluid, and eventually a dipolar molecular condensate.

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The physics of strongly correlated systems in ultracold trapped quantum gases has attracted growing interest recently concerning, in particular, 1D bosonic gases [1], the fractional quantum-Hall effect in rotating Bose gases [2], Bose gases with large scattering lengths [3,4], and the Mott-insulator (MI) to superfluid (SF) phase transition [5] in cold bosonic gases in optical lattices [6,7]. The latter has been recently observed in a remarkable experiment [8].

The physics of ultracold molecular gases is also a very active research area. Cooling and trapping of molecules can be achieved by means of buffer-gas techniques [9], by employing the dipolar moments of polar molecules [10], and by means of photoassociation of ultracold atomic gases [11]. Jaksch *et al.* [12] have recently proposed that a bosonic atomic gas, which is in a MI phase with exactly two atoms per site in an optical lattice, can be used to obtain via photoassociation a superfluid gas of homonuclear molecules, and eventually a molecular Bose-Einstein condensate (BEC).

The influence of dipole-dipole forces on the properties of ultracold gases has also drawn considerable attention. It has been shown that these forces significantly modify the ground state and excitations of trapped dipolar BECs [13–18]. In addition, since dipole-dipole interactions can be quite strong relative to the short-range (contact) interactions, dipolar particles are considered to be promising candidates for the implementation of fast and robust quantum-computing schemes [19,20]. Several sources of cold dipolar bosons have been proposed, including atoms with large magnetic moments [14], and externally induced electric dipoles [13,15,19]. Perhaps the most promising perspective in this sense is provided by ultracold gases of polar molecules with large electric dipole moments, which could eventually dominate the physics of the system [15,16].

This Letter is devoted to the analysis of the generation of ultracold 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 photoassociation, or adiabatic passage. Finally, the quantum melting of the molecular MI into a polar molecular superfluid takes place.

We consider a miscible gas of two trapped atomic bosonic species at very low temperature. Although our calculations could, in principle, be employed for arbitrary atoms, we have assumed below the particular mixture of ^{41}K and ^{87}Rb, whose simultaneous Bose-Einstein condensation has been recently realized [21]. 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. Typically, we employ $\omega_z = 8$ kHz, which guarantees that the transversal wave function can be considered as the (Gaussian) ground state of the harmonic oscillator of frequency ω_z. The physics of the system is governed by the two-species generalization of the Bose-Hubbard (BH) model, described by the Hamiltonian

$$H = \sum_{\langle i,j\rangle}[J_a a_i^\dagger a_j + J_b b_i^\dagger b_j] + U_{ab}\sum_i n_{ai}n_{bi} + \frac{1}{2}\sum_i[U_{0a}n_{ai}(n_{ai}-1) + U_{0b}n_{bi}(n_{bi}-1)], \quad (1)$$

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 $w_a(\mathbf{r}-\mathbf{r}_i)$, $w_b(\mathbf{r}-\mathbf{r}_i)$ 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 minimum of the optical potential as $\mathbf{r}_i$, and the number operator of K (Rb) atoms at the site i as $n_{ai} = a_i^\dagger a_i$ ($n_{bi} = b_i^\dagger b_i$). In

Eq. (1), only the nearest-neighbor tunneling is considered, which is described by the parameter $J_{a,b} = \int w^{\star}_{a,b}(\mathbf{r} - \mathbf{r}_i)[-\frac{\hbar^2}{2m}\nabla^2 + V_l(\mathbf{r})]w_{a,b}(\mathbf{r} - \mathbf{r}_j)d^3r$, where j and i are the indices of neighboring sites, and $V_l(\mathbf{r}) = \sum_{\xi=x,y} V^0_\xi \cos^2(k_\xi \xi)$ is the optical lattice potential (with wave vector $\mathbf{k}$) which we consider to be the same for both species. The optical potential for K and Rb is almost the same for the detunings corresponding to the wavelength 1064 nm of a Nd:Yag laser [22]. The same species interact via a short-range pseudopotential, which is described by the coefficients U_{0a}, U_{0b}: $U_{0a,b} = 4\pi\hbar^2 a_{\mathrm{K,Rb}} \int |w_{a,b}(\mathbf{r} - \mathbf{r}_i)|^4/m_{\mathrm{K,Rb}} d^3r$, where a_{K}, m_{K} (a_{Rb}, m_{Rb}) are the scattering length and atomic mass of potassium (rubidium). The interactions between different species are characterized by the coefficient $U_{ab} = 2\pi\hbar^2 a_{\mathrm{KRb}} \int |w_a(\mathbf{r} - \mathbf{r}_i)|^2 |w_b(\mathbf{r} - \mathbf{r}_i)|^2/m_{ab} d^3r$, where a_{KRb} is the K−Rb scattering length, and m_{ab} is the reduced mass for K and Rb atoms. The scattering length a_{KRb} has been estimated recently to be of the order of 8.6 nm [21]; that is, the repulsive interactions between K and Rb are stronger than those between K-K and Rb-Rb, which are characterized by $a_{\mathrm{K}} = 3.17$ nm and $a_{\mathrm{Rb}} = 5.24$ nm, respectively. As a result, it is energetically favorable for K and Rb particles to remain immiscible, i.e., to stay at different lattice sites, rather than in the same ones. This situation can be, however, modified by means of Feshbach resonances, which can strongly modify the value of a_{KRb} [23]. We have thus assumed that the value of a_{KRb} can be reduced to $0.5\sqrt{a_{\mathrm{K}} a_{\mathrm{Rb}}}$. In that case the two components acquire a miscible phase.

We have considered square lattices up to 80×80 sites, with periodic boundary conditions. In the first stage, we demonstrate the possibility of a transition from a state with two miscible superfluids to a MI phase with exactly one Rb and 1 K atom per site. To this aim we first obtain the ground state using a variational Gutzwiller ansatz [6], $|\Psi_{MF}\rangle = \prod_i |\phi_i\rangle$, where the product is over all lattice sites. The functions $|\phi_i\rangle$ for each site are expressed in the Fock basis, $|\phi_i\rangle = \sum_{n,m=0}^{\infty} f^{(i)}_{n,m} |n, m\rangle_i$, where n, m indicate the occupation number for the K and Rb atoms, respectively. For numerical reasons, we have assumed that maximally three atoms of each species can be present at any lattice site, and checked the validity of this assumption self-consistently. The coefficients $\{f^{(i)}_{n,m}\}$ are found by minimization of $\langle\Psi_{MF}|H - \sum_i[\mu_a n_{ai} + \mu_b n_{bi}]|\Psi_{MF}\rangle$, where the chemical potentials μ_a, μ_b were chosen so that the mean numbers of K, Rb atoms were equal to the number of lattice sites.

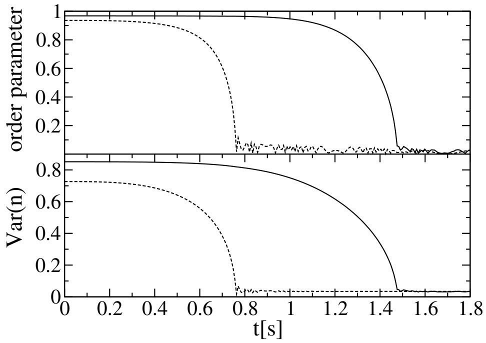

FIG. 1. Dynamical transition from the SF phase of ^{41}K (solid line) and ^{87}Rb (dashed line) atoms to the MI phase. The upper plot shows the value of the order parameters $|\langle a_i\rangle|$, $|\langle b_i\rangle|$ (constant for all lattice sites) for both species, while the lower one depicts the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

The ground state for weak lattice potentials corresponds to the coexistence of superfluids for both species, and it was used as the initial condition for subsequent time-dependent calculations. This state is characterized by a nonvanishing value of the superfluid order parameters $|\langle a_i\rangle|$, $|\langle b_i\rangle|$ (Fig. 1). To drive the system from SF to MI phase, we slowly increase the lattice potential. This process can be described using a dynamical Gutzwiller method, as discussed in Ref. [12]. To this aim, one allows the coefficients $f^{(i)}_{n,m}$ to be time dependent and to follow the dynamics derived from the time-dependent variational principle. The resulting equation becomes

$$\begin{aligned} i\dot{f}^{(i)}_{n,m} = {} & \left[\frac{U_{0a}}{2} n(n-1) + \frac{U_{0b}}{2} m(m-1)\right] f^{(i)}_{n,m} \\ & + J_a[\Phi^{a*}_i \sqrt{n+1} f^{(i)}_{n+1,m} + \Phi^a_i \sqrt{n} f^{(i)}_{n-1,m}] \\ & + J_b[\Phi^{b*}_i \sqrt{m+1} f^{(i)}_{n,m+1} + \Phi^b_i \sqrt{m} f^{(i)}_{n,m-1}] \\ & + U_{ab} nm f^{(i)}_{n,m}, \end{aligned} \tag{2}$$

where $\Phi^a_i = \sum_{\langle i,j\rangle} \langle\Psi_{MF}|a_j|\Psi_{MF}\rangle$ and $\Phi^b_i = \sum_{\langle i,j\rangle} \times \langle\Psi_{MF}|b_j|\Psi_{MF}\rangle$. When the lattice potential increases, the system follows the changes quasiadiabatically, and the two species enter sequentially the MI phase with one atom per site. As shown in Fig. 1, this occurs first for the heavier Rb atoms at $t \approx 0.75$ s, and then at $t \approx 1.5$s for K. The superfluid K introduces random local modifications of the chemical potential for Rb. In our static calculations, this results in a SF to MI transition for Rb at $-U_{0b}/J_b = 25.6$, instead of 23.2, expected for the single-component case. In our dynamical calculations, we obtain the transition at $-U_{0b}/J_b = 26.0$ due to a slight heating. For K, however, the transition occurs when Rb is already in MI. Hence, the presence of Rb just results in a global shift of the chemical potential, and the dynamical transition at $-U_{0a}/J_a = 23.5$ for K just slightly departs due to heating from 23.2.

At the end of the process, each site contains one Rb and one K atom, with relative atom number fluctuations less than 3%. This, however, requires a sufficiently slow modification of the lattice potential, typically within a time scale of 2 sec for a lattice wavelength $\lambda = 1064$ nm.

Note that the time scale is provided by the inverse of the recoil energy of the lattice, and therefore it scales as λ^2. We note also at this point that a transition 3 times faster leads to about 2 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 MI phase with one Rb and one K atom per site, a heteronuclear molecule can be generated at each lattice site. One possible method 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 $\Omega = 0^+$ or 1 symmetry, where Ω labels projection of 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 ${}^1\Sigma^+$ 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 $1/R^3$ 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 deexcitation step [24]. In any case, our preliminary calculations indicate that favorable paths for photoassociation should be feasible. 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 a.u. (1 a.u. is 8.478×10^{-30} C m), whereas it is much larger, 0.30 a.u., for the ${}^1\Sigma^+$ $v = 0$ level [25]. In the latter case, special care should be taken to prevent the heating due to blackbody 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 in the z direction by an external electric field ($\approx$100 V/cm), we have to include the dipole-dipole interactions in our calculations. The Hamiltonian reads [7]

$$H = J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{1}{2} U_0 \sum_i n_i(n_i - 1) + \frac{1}{2} U_{\sigma_1} \sum_{\langle i,j \rangle} n_i n_j + \frac{1}{2} U_{\sigma_2} \sum_{\langle\langle i,j \rangle\rangle} n_i n_j + \ldots, \tag{3}$$

where b_i is the annihilation operator of a heteronuclear molecule at the lattice site i. The number operator n_i, the Wannier basis $w(\mathbf{r} - \mathbf{r}_i)$, and the tunneling coefficient J for molecules are defined similarly as in Eq. (1) [26]. However, the interaction part significantly differs from that of Eq. (1). The coefficients U_σ are defined as follows: $U_\sigma = \int |w(\mathbf{r} - \mathbf{r}_i)|^2 V_{\rm int}(\mathbf{r} - \mathbf{r}') |w(\mathbf{r}' - \mathbf{r}_j)|^2 \, d^3r \, d^3r'$, where $\sigma = |\mathbf{r}_i - \mathbf{r}_j||\mathbf{k}|/4\pi$ is the dimensionless intersite distance. In particular, U_0 determines the on-site interactions, U_{σ_1} the nearest-neighbor interactions, U_{σ_2} the interactions between the next-nearest neighbors, etc. Consequently, the respective summations in Eq. (3) must be carried out over appropriate pairs of sites which are marked by $\langle \cdots \rangle$ for the nearest neighbors, $\langle\langle \cdots \rangle\rangle$ for the next-nearest neighbors, etc. In the 2D calculations presented below, we have taken into account interactions with up to four neighbors ($\sigma_1 = 1$, $\sigma_2 = \sqrt{2}$, $\sigma_3 = 2$, $\sigma_4 = \sqrt{5}$), since the effects of interactions of a longer range are negligible. For polarized dipoles, the interaction potential is

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

where the first part of Eq. (4) provides the dipole-dipole interaction characterized by the dipole moment d and the angle θ between the dipole direction and the vector $\mathbf{r} - \mathbf{r}'$. 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. [25], and assume the s-wave scattering length of K-Rb molecule as $a = \sqrt{a_{\rm K} a_{\rm Rb}}$ [27].

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 MI 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 (3). 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 relatively fast since

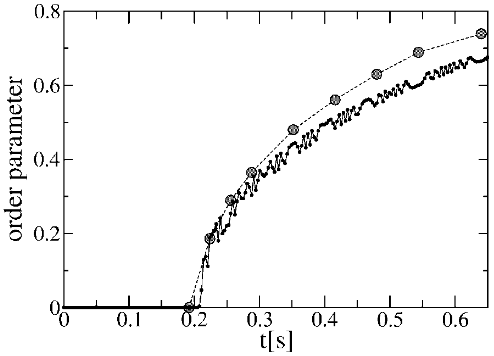

FIG. 2. Melting of ^{41}K–^{87}Rb dimers initially in the MI phase. The plot shows the time evolution of the molecular superfluid order parameter $|\langle b_i \rangle|$ (solid line), which is the same for all lattice sites. The dashed line refers to static calculations of the ground state of the dipolar molecules placed in the lattice. Note a very sharp transition from the MI phase to the SF one, that occurs at $t \approx 0.2$ s. The frequency of the transverse confinement was changed as $\omega_z(t) = \omega_{\rm MI} + (\omega_{\rm SF} - \omega_{\rm MI})t/t_0$, where $\omega_{\rm MI}/2\pi = 8$ kHz, $\omega_{\rm SF}/2\pi = 6$ kHz, and $t_0 = 0.65$ s.

the MI gap guarantees the adiabaticity at this stage. In a second (relatively slower) stage, we have found it more convenient to modify the transversal confinement. As shown in Refs. [7,15], the properties of the dipolar gas strongly depend on the aspect ratio of the on-site wave function. In particular, by reducing the transverse confinement, the on-site wave function becomes more elongated in the transverse direction. As a consequence, U_0 decreases [7], and the system enters into the SF phase. Figure 2 shows this process. Because of the noncompletely adiabatic evolution, the gas does not exactly follow the expected stationary result, although very clearly a SF molecular phase is accomplished. The ratio $-U_0/J \approx 23.2$ at which the transition from MI to SF is close to the value expected for a 2D single-component gas without a permanent dipole moment, because at the transition point the ratios U_σ/U_0 are small. As shown in Fig. 2, this dynamical transition into the SF phase occurs for realistic parameters in a time scale of 1 s. This transition can be realized, 50 times faster, although the dynamics is in such a 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 photoassociated 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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[23] The scattering models are not yet good enough to predict the specific magnetic fields for the resonances, but they will undoubtedly exist for field strengths below a few hundred Gauss for a molecule with a mass as heavy as KRb. This argument is supported by our estimations based on the asymptotic level structure.
[24] Also, the on-site densities ($\approx 10^{15}$ cm^{-3}) are 10 000 times larger than in traditional photoassociation experiments.
[25] P. Julienne and S. Kotochigova (to be published).
[26] We assume that the laser forming the lattice is far off-resonant for both atoms and molecules, so that the resulting potentials are similar for both of them.
[27] 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.