# Controlling two-species Mott-insulator phases in an optical lattice to form an array of dipolar molecules 

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#### Abstract

We consider the transfer of a two-species Bose-Einstein condensate (BEC) into an optical lattice with a density such that a Mott-insulator state with one atom per species per lattice site is obtained in a deep lattice regime. Depending on collisional and transition parameters, the result could be either a "mixed" or a "separated" Mott-insulator phase. Such a mixed two-species insulator would be well suited for the formation of dipolar molecules via photoassociation. The resulting array of dipolar molecules could then be used for the formation of a dipolar molecular condensate or for computation. For the case of a ${ }^{87} \mathrm{Rb}-{ }^{41} \mathrm{~K}$ two-species BEC, however, the large interspecies scattering length makes it difficult to obtain the desired mixed Mott-insulator phase. To overcome this difficulty, we investigate the effect of varying the lattice frequency on the mean-field interaction and propose a favorable parameter regime, under which a lattice of dipolar molecules could be generated.


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In a ground-breaking recent experiment, a quantum phase transition from a superfluid (SF) to a Mott-insulator (MI) state was observed by varying the depth of a threedimensional (3D) optical lattice superimposed onto a trapped Bose-Einstein condensate (BEC) of ${ }^{87} \mathrm{Rb}$ atoms [1]. This experiment highlights a growing trend in ultracold atomic physics whereby condensates are no longer the direct object of study, but serve mainly as well-controlled initial state for the preparation of more exotic highly-correlated many-body states. In addition to providing a new insight into fundamental phenomena of condensed-matter physics, MI states are expected to have important applications in Heisenberglimited atom interferometry [2] and quantum computing [3,4].

An additional interesting application of a Mott insulator was recently proposed by Jaksch and co-workers: employing a Mott-insulator state as an intermediate stage in the generation of a BEC of molecules [5]. Molecules would be formed via stimulated Raman photoassociation of a Mott insulator with two atoms per lattice site, resulting in a molecular MI with unit filling factor that could then be "melted" (by adiabatically reducing the lattice depth) to form a molecular BEC. This is a distinct advantage over photoassociation in the superfluid phase [6,7], as photoassociation strongly favors the creation of vibrationally excited molecules-due to favorable Franck-Condon transition from the continuumwhich tend to undergo inelastic collisions in the presence of other atoms and/or molecules. In such a collision, the resulting release of vibrational quanta leads to loss of both particles from the trap. The primary advantage of the Mottinsulator approach is thus the fact that during photoassociation the resulting molecules would be completely isolated from collisions with other atoms and/or molecules. By isolating each vibrationally excited molecule in a

[^0]lattice site, it should be possible to stimulate the molecules into the ground rotational-vibrational state before melting the Mott insulator, thus eliminating this collisional loss mechanism.

In this Rapid Communication, we extend this idea to the formation of a lattice of two-species Mott-insulator phase with precisely one atom per species per lattice site. This scheme would require a two-species Bose-Einstein condensate as a starting point, as has been recently demonstrated with ${ }^{87} \mathrm{Rb}$ and ${ }^{41} \mathrm{~K}[8,9]$. The two-species condensate would then be adiabatically loaded into a three-dimensional optical lattice, resulting in the formation of either a mixed or separated MI state, corresponding to each lattice site containing different or identical species, respectively, see Fig. 1. The formation of a mixed phase turns out to be difficult for the case of a ${ }^{87} \mathrm{Rb}^{-}{ }^{41} \mathrm{~K}$ system due to the large repulsive interspecies scattering length, which favors the separated phase. We propose overcoming this difficulty by varying the optical lattice frequency, which exploits the difference in atomic resonance frequencies to control the relative densities of the two species.

Preparing a Mott-insulator state of heteronuclear molecules by this approach would be an effective method to obtain a lattice of dipolar molecules for use as a qubit register in a quantum computer [10]. In addition, a rich variety of quantum phases are predicted for the ground state of a lattice of dipolar bosons, including a supersolid phase [11]. Once formed, the lattice of dipolar molecules could also be melted by adiabatically lowering the lattice potential, resulting in a condensate of dipolar bosons. Here the long-range dipoledipole interactions should introduce interesting correlations effect in both the ground state and collective excitations of the BEC [12-16].

Others have considered the related problem of superfluidinsulator transitions for spinor (multicomponent) BECs [17] in which the added freedom of superpositions of hyperfine states is included. One crucial difference between a twospecies system and a spinor system is the fact that each atomic species will see a different optical potential as a result


FIG. 1. (Color online) Separated- (left) and mixed- (right) two-species Mott-insulator phases in an optical lattice. The separated-phase MI is randomly distributed.
of having different dipole moments and resonance frequencies. This additional freedom should result in the physics of a two-species system being significantly richer than that of a single-species spinor system. For example, due to the potential for different tunneling rates between neighboring lattice sites and/or collision rates for each species, the superfluidinsulator transition will most likely occur at a different lattice intensity for each species, resulting in a regime where an MI of one species is embedded in an SF of another species. Thus, the phases of a dual-species lattice can be divided into three categories: a dual SF, a hybrid SF-MI phase, and a dual MI phase. At present we will focus primarily on the properties of the dual MI phase as it is the only phase with the potential for collisionless photoassociation into dipolar molecules.

The starting point for our theoretical consideration is a two-species atomic system in the presence of an optical lattice potential. The atomic density is assumed to be such that at the center of the trap, there is one atom per species per cubic wavelength. Our discussion will apply to either 1D, 2 D , or 3 D lattices, provided that tight confinement is provided in the additional dimensions. The Bose-Hubbard Hamiltonian [18] that describes such a system is then given by

$$
\begin{align*}
\hat{H}= & \frac{\hbar}{2} \sum_{j}\left[g_{11} \hat{n}_{1 j}\left(\hat{n}_{1 j}-1\right)+g_{22} \hat{n}_{2 j}\left(\hat{n}_{2 j}-1\right)+2 g_{12} \hat{n}_{1 j} \hat{n}_{2 j}\right] \\
& +\hbar \sum_{i, j}\left[\beta_{1 i j} \hat{c}_{1 i}^{\dagger} \hat{c}_{1 j}+\beta_{2 i j} \hat{c}_{2 i}^{\dagger} \hat{c}_{2 j}\right] \tag{1}
\end{align*}
$$

where $\hat{c}_{i j}$ is the bosonic annihilation operator for species $i$ at lattice site $j, \hat{n}_{i j}=\hat{c}_{i j}^{\dagger} \hat{c}_{i j}$ is the corresponding number operator, $\beta_{i j k}$ is the rate of tunneling of species $i$ from lattice site $j$ to site $k$, and $g_{i j}$ is the collision rate for collisions between species $i$ and $j$. In this work we will concentrate on controlling the collision parameters $g_{i j}$ by varying the control parameters of the optical lattice. We note that the tunneling terms can also be controlled by the same mechanism, but are not of interest in the present treatment as our conclusions are drawn exclusively from the relative strength of the collision terms.

In order to compute the various interaction coefficients, we must first consider the dependence of the optical lattice potential on the intrinsic properties of each atomic species. The optical potential seen by species $i$ can be expressed as

$$
\begin{equation*}
V_{i}(\mathbf{r})=\frac{d_{i}^{2}}{\left(\omega_{i}-\omega_{L}\right)} U(\mathbf{r}) \tag{2}
\end{equation*}
$$

where $d_{i}$ and $\omega_{i}$ are the dipole moment and resonance frequency of species $i$, respectively, $\omega_{L}$ is the laser frequency of the optical field, and $U(\mathbf{r})=-|E(\mathbf{r})|^{2} / \hbar$ is the speciesindependent intensity of the optical field. Assuming that the sign of detuning is the same for both species, in which case the potential minima will coincide, we can expand an arbitrary lattice site around the potential minima according to $U(\mathbf{r})=u_{0}+\frac{1}{2} \Sigma_{\mu} u_{\mu} r_{\mu}^{2}$, giving

$$
\begin{equation*}
V_{i}(\mathbf{r})=\frac{1}{2} \frac{d_{i}^{2}}{\left(\omega_{i}-\omega_{L}\right)} \sum_{\mu} u_{\mu} r_{\mu}^{2} \tag{3}
\end{equation*}
$$

where we have dropped the constant term, consistent with a transformation to a rotating frame which leaves the Hamiltonian (1) unchanged. The Cartesian coordinates, defined for each identical lattice well $i$ are denoted by $r_{\mu}$, where the potential minimum is taken as the origin and $\mu=x, y, z$.

Following the expansion in Eq. (3), we make a Gaussian approximation for the lowest-energy Wannier modes of a lattice site for species $i$ as

$$
\begin{equation*}
\phi_{i}(\mathbf{r})=\pi^{-3 / 4} \prod_{\mu} \lambda_{i \mu}^{-1 / 2} e^{-(1 / 2)\left(r_{\mu} / \lambda_{i \mu}\right) 2 / 2} \tag{4}
\end{equation*}
$$

where we have introduced the harmonic-oscillator length for species $i$ along the direction $\hat{r}_{\mu}$,

$$
\begin{equation*}
\lambda_{i \mu}=\left[\frac{\hbar^{2}\left|\omega_{i}-\omega_{L}\right|}{m_{i} d_{i}^{2} u_{\mu}}\right]^{1 / 4} \tag{5}
\end{equation*}
$$

$m_{i}$ being the atomic mass of species $i$. With these wave functions, we can compute the collision coefficients via

$$
\begin{align*}
g_{i j} & =\frac{2 \pi \hbar a_{i j}}{\mu_{i j}} \int d \mathbf{r}\left|\phi_{i}(\mathbf{r})\right|^{2}\left|\phi_{j}(\mathbf{r})\right|^{2} \\
& =\frac{2 \hbar a_{i j}}{\sqrt{\pi} \mu_{i j}} \prod \frac{1}{\sqrt{\lambda_{i \mu}^{2}+\lambda_{j \mu}^{2}}} \tag{6}
\end{align*}
$$

where $a_{i j}$ is the scattering length for collisions between species $i$ and $j$ and $\mu_{i j}=m_{i} m_{j} /\left(m_{i}+m_{j}\right)$ is the reduced mass the two-species system.

Since the harmonic-oscillator length (5) for a given atomic species tends to zero when approaching the atomic resonance frequency, tuning the lattice frequency close to the resonance frequency of one atomic species can act as a strong "handle" with which to tune the relative atomic densities, and hence the collision parameters of the system. The


FIG. 2. (Color online) Relative density parameter in an optical lattice for ${ }^{23} \mathrm{Na},{ }^{41} \mathrm{~K}$, and ${ }^{87} \mathrm{Rb}$ as a function of the lattice frequency $\omega_{L}$. The relative density parameter is in units of $\left[m_{p} e^{2} a_{0}^{2} / c R_{\infty}\right]^{3 / 4}$ and the laser frequency is in units of $c R_{\infty}$.
local density per atom, defined as $1 / V_{i}=\Pi_{\mu} \lambda_{i \mu}^{-3}$, is given by $1 / V_{i}=\rho_{i} \hbar^{-3 / 2} \Pi_{\mu} u_{\mu}^{3 / 4}$, where we have introduced the relative density parameter

$$
\begin{equation*}
\rho_{i}=\left[\frac{m_{i} d_{i}^{2}}{\left|\omega_{L}-\omega_{i}\right|}\right]^{3 / 4} . \tag{7}
\end{equation*}
$$

The ratio of the local densities for the different species, $V_{i} / V_{j}=\rho_{j} / \rho_{i}$ is independent of the lattice parameters $u_{\mu}$, provided only that the wells are sufficiently deep such that the Gaussian approximation holds for the lowest Wannier state-generally valid when the lattice depth is large as compared to the atomic recoil energy. In Fig. 2, we plot the dimensionless density parameter $\rho_{i}$ as a function of $\omega_{L}$ for atomic species currently used in BEC experiments: ${ }^{23} \mathrm{Na}$, ${ }^{41} \mathrm{~K}$, and ${ }^{87} \mathrm{Rb}$. From this figure, we note that a wide range of relative densities can be obtained by varying the lattice frequency across the atomic resonance frequencies. The atomic parameters in this calculation are

$$
\begin{gathered}
m_{i}=\{22.99,40.96,86.91\} m_{p}, \\
\omega_{i}=\{0.9720,0.7472,0.7351\} c R_{\infty},
\end{gathered}
$$

and $d_{i}=\{0.9036,0.8227,0.8023\} e a_{0}$, respectively, where $m_{p}$ is the proton mass, $e$ the electron charge, $a_{0}$ the Bohr radius, $c$ the speed of light, and $R_{\infty}$ the Rydberg constant. In analogy with previous studies of Bose-Hubbard Hamiltonians [11, 17,18], it is safe to assume that for a deep enough lattice and for strictly positive-scattering lengths, the ground state of the two-species Bose-Hubbard model having $N$ atoms per species and $N$ lattice sites will be an insulator state, i.e., the atoms will be localized in individual wells. The minimumenergy arrangement of the two atomic species then depends on the relative strengths of interspecies and intraspecies collision parameters. In principle, there is a broad variety of possible two-species Mott-insulator phases. If, e.g., one species has an extremely weak self-interaction relative to the other interaction parameters, then it may be energetically favorable for all atoms of the first species to occupy a single lattice site with the second species uniformly distributed over


FIG. 3. (Color online) The ratio of the energies per particle of the separated and mixed phases of a ${ }^{87} \mathrm{Rb}-{ }^{41} \mathrm{~K}$ two-species Mott insulator as a function of the lattice frequency $\omega_{L}$ taken in units of $c R_{\infty}$.
the remaining sites. We do not consider such extreme situations and instead focus on the more likely regime where the ground state contains exactly two atoms per site. This regime has two phases: a mixed phase where one atom per species occupies each site, and a separated phase where each site contains two atoms of the same species. We note that the separated phase is unique since in that the ground state could be any quantum superposition of different patterns for distributing the two species.

The collisional energy per lattice site of the MI state is given by $E_{s, m}=(1 / N)\left\langle\psi_{m, s}\right| \hat{H}\left|\psi_{s, m}\right\rangle$, where $N$ is the number of lattice sites. For the case of two lattice sites, the quantum state of the separated MI phase is

$$
\begin{equation*}
\left|\psi_{s}\right\rangle=\frac{1}{2} \hat{c}_{11}^{\dagger} \hat{c}_{11}^{\dagger} \hat{c}_{22}^{\dagger} \hat{c}_{22}^{\dagger}|0\rangle, \tag{8}
\end{equation*}
$$

whereas the ground state of the mixed MI phase is

$$
\begin{equation*}
\left|\psi_{m}\right\rangle=\hat{c}_{11}^{\dagger} \hat{c}_{12}^{\dagger} \hat{c}_{21}^{\dagger} \hat{c}_{22}^{\dagger}|0\rangle \tag{9}
\end{equation*}
$$

The energy per lattice site calculated from this two-site state will remain valid as the lattice is scaled up to any even number of sites. The energy per lattice site for the separated phase is $E_{s}=\frac{1}{2}\left(g_{11}+g_{22}\right)$, whereas the energy of a pair of mixed-phase per lattice site is $E_{m}=g_{12}$. The condition for a mixed-species ground state is therefore $E_{s} / E_{m}=\left(g_{11}\right.$ $\left.+g_{22}\right) / 2 g_{12}>1$, which can be determined with the help of Eqs. (5) and (6).

In Fig. 3, we plot this ratio as a function of the lattice frequency $\omega_{L}$ for the case of ${ }^{87} \mathrm{Rb}$ and ${ }^{41} \mathrm{~K}$. We use the scattering length data $a_{R b-R b}=99 a_{0}, a_{K-K}=60 a_{0}$, and $a_{R b-K}=163 a_{0}$, taken from the recent report on a twospecies superfluid [9]. The frequency domain is divided into five regions. In region I, both species see a red-detuned lattice and the ground state is a separated dual MI. In region II, which spans from $\omega_{L}=0.733663$ to the ${ }^{87} \mathrm{Rb}$ resonance, both species also see a red-detuned lattice but the increase in the rubidium density results in the ground state being the desired mixed phase. Since the mean-field energy is proportional to $\rho_{i}^{2}$, there is an additional energy cost associated with having Rb atoms at the same lattice site. Region III lies between the Rb and K resonances, and hence the two species
see different potential minima, e.g., $g_{i j} \approx 0$ for $i \neq j$. Here the ground state will be a dual MI, but with the Rb atoms localized at the lattice intensity minima and the K atoms localized at the intensity maxima. In regions IV, which spans from the K resonance frequency to $\omega_{L}=0.747631$ and V , both species see a blue-detuned lattice, with region IV corresponding to a mixed phase and region V to a separated phase.

The mixed phase occurs only in the vicinity of an atomic resonance; thus, we must make sure that spontaneous emission rates are sufficiently small and remain negligible for experimentally realizable time scales. By integrating over the lattice intensity via

$$
\int d z\left\{\begin{array}{c}
\cos ^{2}(k z) \\
\sin ^{2}(k z)
\end{array}\right\} \times e^{-z^{2}}=\frac{\sqrt{\pi}}{2}\left(1 \pm e^{-k^{2}}\right)
$$

and the help of Eqs. (2)-(5), it can be determined that the spontaneous emission rate of an atom in the ground state of a spherically symmetric lattice well with depth $\alpha \hbar \omega_{R}, \omega_{R}$ $=\hbar \omega_{L}^{2} /\left(m_{i} c^{2}\right)$ being the atomic recoil frequency, is given in the Gaussian approximation by

$$
\begin{equation*}
\gamma_{i}=\frac{3}{2} \alpha \omega_{R} \frac{\Gamma_{i}}{\left|\omega_{i}-\omega_{L}\right|}\left(1 \pm e^{-1 / \sqrt{\alpha}}\right), \tag{10}
\end{equation*}
$$

where $\Gamma_{i}$ is the natural linewidth of species $i$ and the + and - signs give the result for a red-detuned and a blue-detuned lattice, respectively. For ${ }^{87} \mathrm{Rb}$, with $\Gamma_{R b}=5 \mathrm{MHz}$, we find that the average decay rate just to the right of the I-II boundary is $\gamma_{R b} \approx \alpha\left(1+e^{-1 / \sqrt{\alpha}}\right) \times 7 \times 10^{-2} \mathrm{~Hz}$, which for $\alpha=20$ gives a lifetime per atom of 0.38 s . Similarly, on the bluedetuned side, we find the average decay rate for ${ }^{41} \mathrm{~K}$, with $\Gamma_{K}=6 \mathrm{MHz}$, just to the left of the IV-V boundary is given by $\gamma_{K} \approx \alpha\left(1-e^{-1 / \sqrt{\alpha}}\right) \times 7 \times 10^{-1} \mathrm{~Hz}$. For $\alpha=20$, this gives a lifetime per $K$ atom of 0.35 s , roughly the same as for Rb .

The time scale for adiabatic passage from an SF to an MI state is typically of the order of 10 ms , so working in either the red (II)- or blue (IV)-detuned regions should be feasible without spontaneous heating. We note that once the mixed dual-MI state is reached, the lattice depth could be ramped to a large enough value to suppress tunneling, after which the lattice frequency could be moved much further away from the atomic resonance while preserving the mixed dual-MI state as a metastable state. With this technique, the mixed phase could have a much longer spontaneous lifetime to facilitate more time consuming photoassociation or quantumcomputing processes.

In conclusion, we have determined the ground-state configuration of a two-species optical lattice for the case where the number of atoms in each species equals the number of lattice sites, showing that varying the lattice frequency leads to a variety of MI phases. In making the transition to a dual-MI state from a dual-SF state, it is likely that each species will undergo the superfluid-insulator transition at a different lattice intensity, passing through a potentially interesting hybrid SF-MI state. While there are no obvious difficulties in reaching the mixed dual-MI state in this manner, dynamical simulation of the Bose-Hubbard model with the exact Wannier states is needed to ensure that the system can indeed be driven into the true ground state, a task we plan to carry out in a future work.

Note added. Recently, we became aware of a related manuscript by Damski et al. [19] which reaches similar conclusions but concentrates on different aspects of the proposed technique.

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