

A staggered dual Mott insulator in a 3D optical lattice

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We propose a novel scheme for trapping ultracold rubidium and ytterbium atoms in a three-dimensional (3D) optical lattice simultaneously, in which the two species of atoms locate on two staggered lattices with the same spatial period and have a spatial separation of 133 nm. Furthermore, we calculate the tunneling and intra- and interspecies interactions of rubidium and ytterbium atoms as a function of light intensity, and find that the mixture of quantum degenerate gases in optical lattices can exhibit more intriguing quantum phases, especially a staggered dual Mott insulator of alkali-metal and alkaline-earth metal atoms.

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Ultracold atoms in optical lattices have proven to be a versatile model system to simulate complex quantum phases and investigate unsolved many-body problems from condensed-matter physics in a highly controllable fashion^[1–3]. As an outstanding example, phase transition of superfluid (SF) to Mott insulator (MI) has been predicted theoretically^[4] and observed experimentally^[3]. In addition, ultracold multi-flavor gases offer new insight into the atomic interspecies interaction and ultracold molecule^[5–7]. Recently, the mixtures of bosonic and fermionic atoms in optical lattices have draw much attention due to the occurrence of complex quantum phases, such as phase separation^[8], supersolid phase^[9], and unexpected large shift of the phase transition^[10]. Up to now, experimental efforts to load two-species alkali-metal atoms in an optical lattice have succeeded in several groups^[11–14]. The mixture of alkali-metal and alkaline-earth(-like) atoms has been also investigated, such as rubidium (Rb)-ytterbium (Yb)^[15,16] and lithium (Li)-Yb^[17,18]. In this paper, more unexpected phases have been theoretically predicted and investigated experimentally. Especially, the appearance of a dual MI of bosons and fermions is a paradigmatic example of this diversity^[6].

In this letter, we propose a novel scheme to trap both ⁸⁷Rb and ¹⁷⁴Yb atoms in a staggered three-dimensional (3D) lattice with a laser field, and predict a new dual MI of the mixture of alkali-metal and alkaline-earth atoms, which is greatly different from the dual MI realized by Takahashi group in Kyoto University^[6]. Experimental realization is also discussed.

Now we begin to describe the scheme in detail. First, a two-flavor quantum degenerate gas of Rb and Yb atoms is prepared^[15,16]. Then a laser at 532 nm is used to produce a 3D lattice, which is red-detuned for ¹S₀ to ¹P₁ transition of Yb atoms but blue-detuned for D line transitions of Rb atoms. Therefore, the Rb and Yb atoms

are trapped in the regions of the minimum and maximum light intensity, respectively, and lattice potentials of Rb and Yb atoms can be written as

$$V_{\text{Rb}} = V_{\text{Rb}} \cos^2(kx), \quad (1)$$

$$V_{\text{Yb}} = V_{\text{Yb}} \sin^2(kx), \quad (2)$$

where k and $V_{\text{Rb/Yb}}$ describe the wave vector and the potential depth of Rb/Yb atoms, respectively.

From Eqs. (1) and (2), we plotted the sketch of one dimensional (1D) potentials in Fig. 1. The lattice potentials for two species have equal spatial periods (266 nm) but staggered with a spatial separation of 133 nm. It is clear that the lattice depth of Yb atoms is larger than that of Rb atoms, which is in accordance with our calculation on lattice depth below. To obtain the trap depth of the mixture in an optical lattice, we use the following expressions^[19]

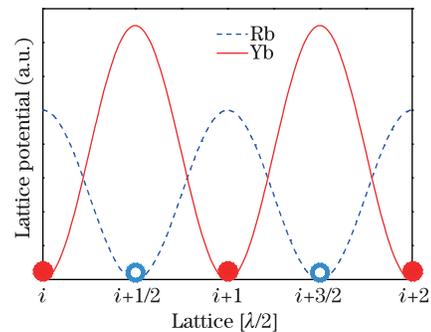


Fig. 1. Light potentials for Rb and Yb atoms in a staggered optical lattice. The solid and hollow balls depict the Rb and Yb atoms, respectively. The dash and solid lines represent the potential experienced by Rb and Yb atoms, respectively. They are staggered with a spatial separation of 133 nm.

$$V_{\text{Rb}} = 4 \times \frac{-3\pi c^2 I}{2} \left[f_{D1} \frac{\Gamma_{D1}}{\omega_{D1}^3} \left(\frac{1}{\omega_{D1} - \omega} \frac{1}{\omega_{D1} - \omega} \right) + f_{D2} \frac{\Gamma_{D2}}{\omega_{D2}^3} \left(\frac{1}{\omega_{D2} - \omega} \frac{1}{\omega_{D2} - \omega} \right) \right], \quad (3)$$

$$V_{\text{Yb}} = 4 \times \frac{-3\pi c^2 I}{2} \frac{\Gamma}{\omega_0^3} \left(\frac{1}{\omega_0 - \omega} \frac{1}{\omega_0 - \omega} \right), \quad (4)$$

where the factor 4 is introduced for optical lattices. f_{D1} (f_{D2}) is the oscillation strength of Rb atom D1 (D2) line. Γ and Γ_{D1} (Γ_{D2}) are the spontaneous decay rate of Yb 1P_1 state and Rb atom $^2P_{1/2}$ ($^2P_{3/2}$) state, respectively. ω_0 and ω_{D1} (ω_{D2}) describe the resonance frequency of Yb $^1S_0 \rightarrow ^1P_1$ state and Rb atom D1 (D2) line, respectively. For Yb atoms, we only consider the $^1S_0 \rightarrow ^1P_1$ transition, which has a wavelength of 399 nm and a spontaneous decay rate of 175.4 MHz^[20], because the spontaneous decay rates of other transitions are far smaller and neglectable. While for Rb atoms, both D1 and D2 line transitions should be considered.

It is shown in Fig. 2 that the atoms of both species experience the different lattice potentials and thus lattice depths are different. Here the waist of the lattice laser is set to 100 μm and the recoil energies $E_{r,\text{Rb}} = \frac{\hbar^2 k^2}{2m_{\text{Rb}}}$ and $E_{r,\text{Yb}} = \frac{\hbar^2 k^2}{2m_{\text{Yb}}}$ are chosen to be the units of the trap depths, respectively. Because the frequency of the lattice light is between the resonant transition frequencies of the Rb and Yb atoms, the signs of the laser-atom detunings are even opposite at the maximum/minimum of light intensity which make it impossible to trap them at the same site. The Rb atoms experience a blue-detuned lattice potential and thus are located at the minimum of the light intensity, while a red-detuned lattice collects the Yb atoms at the maximum of the light intensity. Therefore a staggered optical lattice for trapping the mixture of quantum gases is formed. The most advantage of our proposal is that the staggered lattice can trap both species of the mixture simultaneously and the trap depths can be also adjusted conveniently since only the intensity of 532 nm laser needs to be changed. Very recently, a complicated Mott-insulator phase, named as the dual MI, has been found in the mixture of Yb isotopes^[6]. Naturally, one can expect that the present setup can be used to realize more novel phases related to MI. We have estimated that for a lattice light of the power of 0.5 W, the depths

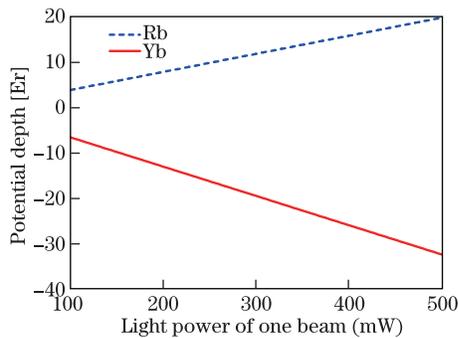


Fig. 2. Potential depth of both species varying with the power of 532-nm laser. Since the Rb and Yb atoms experience red-detuned and blue-detuned lattice potentials, respectively, the signs of their depths are opposite.

of both atoms can be reached to 20 $E_{r,\text{Rb}}$ and 32 $E_{r,\text{Yb}}$, respectively, which is deep enough to freeze the tunneling of the atoms simultaneously. We name the novel phase as the staggered MI due to our special lattice configuration. It should be noted that the predicted phase here is completely different from the existing insulating phases of quantum mixtures, where the atoms of different species are located and interacted locally at each site.

This quantum degenerate mixture gases in an optical lattice can be well described by the extended Bose-Hubbard model

$$\begin{aligned} \hat{H} = & -z \sum_{\langle i,j \rangle} (J_{\text{Rb}} \hat{b}_i^\dagger \hat{b}_j + J_{\text{Yb}} \hat{c}_i^\dagger \hat{c}_j) \\ & + \frac{U_{\text{Rb}}}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{U_{\text{Yb}}}{2} \sum_i \hat{m}_i (\hat{m}_i - 1) \\ & + z U_{\text{RbYb}} \sum_i \hat{n}_{i+\frac{1}{2}} \hat{m}_i, \end{aligned} \quad (5)$$

where $z = 6$ for a 3D lattice and $\langle i,j \rangle$ indicates the nearest neighbor sites on the respective lattices. $J_{\text{Rb/Yb}}$, $U_{\text{Rb/Yb}}$, and U_{RbYb} represent the tunneling, intra- and interspecies interaction energies, respectively. \hat{b}_i (\hat{c}_i) is the annihilation operator while $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ ($\hat{m}_i = \hat{c}_i^\dagger \hat{c}_i$) denotes the number operator for Rb (Yb) atoms at the site i . Next we begin to check the tunneling, intra- and interspecies interaction energies at different light powers, which is of great importance for characterizing many-body phases of the atoms in optical lattices. The parameters are given by^[21]

$$J_{\text{Rb/Yb}} = \frac{\max(E_q^0 - \min(E_q^0))}{4}, \quad (6)$$

$$U_{\text{Rb/Yb}} = \frac{4\pi a_{s\text{Rb/Yb}} \hbar^2}{m} \int d^3x |w_{\text{Rb/Yb}}(x)|^4, \quad (7)$$

$$U_{\text{RbYb}} = \frac{4\pi a_{s\text{RbYb}} \hbar^2}{\mu} \int d^3x |w_{\text{Rb}}(x)|^2 |w_{\text{Yb}}|^2, \quad (8)$$

where E_q^0 represents the eigenenergy of the ground band. The scattering lengths $a_{s\text{Rb}} = 102a_0$, $a_{s\text{Yb}} = 105a_0$, and $a_{s\text{RbYb}} = 83a_0$ have been used with a_0 of the Bohr's radius. $w_{\text{Rb/Yb}}$ and $\mu = m_{\text{Rb}}m_{\text{Yb}}/(m_{\text{Rb}} + m_{\text{Yb}})$ represent the Wannier function and the reduced mass, respectively. The calculated results are depicted in Fig. 3.

With increasing the power of the lattice light at 532 nm, the depths of both species increase and result in a larger interaction energy for the atoms at each lattice site and a smaller tunneling rate between neighbor sites. Especially, because the lattice depth of the Rb atoms is smaller that of the Yb atoms at an arbitrary light power, $U_{\text{Rb}} < U_{\text{Yb}}$ and $J_{\text{Rb}} < J_{\text{Yb}}$ can be always satisfied. In addition, we also found that the interspecies interaction energy U_{RbYb} is very small and neglectable which originates from the negligible overlap of the wavefunctions of Rb and Yb atoms in staggered neighbor sites. Therefore, the total Hamiltonian (Eq. (5)) can be reduced to the superposition of two independent standard Bose-Hubbard Hamiltonians.

This means that it is possible to freeze both species at their respective sites and reach to a MI phase with a

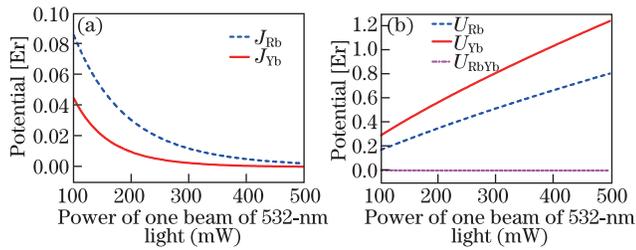


Fig. 3. (a) Tunneling energies of Rb and Yb atoms depend on the power of the 532-nm laser; (b) intra- and interspecies interaction energies of Rb and Yb atoms depend on the power of the 532-nm laser. The interspecies interaction are far smaller than the tunneling and intraspecies interaction when the power larger than 50 mW.

Table 1. Critical Power of Phase Transition

	Critical Potential Depth	Critical Power (mW)	Critical Intensity (kW/cm ²)
Rb	$12E_{r,Rb}$	288	1.83
Yb	$11E_{r,Yb}$	174	1.11

staggered spatial distribution at the zero-tunneling regime. As is well known, the critical point of SF-MI transition in a 3D lattice is $U/J = 34.8$ in the first lobe^[22]. Accordingly, we found out the critical values of light intensity for the Rb and Yb atoms as shown in Table 1.

From the above table, one can conclude that the mixture of two species in an optical lattice can be evolved into three different phases which correspond to different intensities of the lattice light. Starting from a two-species BEC of the Rb and Yb atoms, one can increase the intensity of the lattice light gradually and load the Yb atoms in the lattice first. It is apparent that the Yb atoms take the lead in transforming from SF to insulating phase because of a lower critical value of phase transition (1.11 kW/cm²). At this time, the mobile SF phase of the Rb atoms and the frozen insulating phase of the Yb atoms coexist. Furthermore, when the power of the lattice laser is larger than 1.83 kW/cm², a more interesting phase emerges in which two independent MIs are presented and staggered from each other in space. In this dual MI phase, the dynamics of the atoms of two species are both governed by the intra-species interactions.

Finally we briefly discuss experimental realization of our scheme. In recent years, the mixture of cold Rb and Yb atoms have been realized^[15,16], and the 532-nm laser has power up to 18 W^[23], which allowing ones for detailed studies of its properties in the experiment. In addition, the mass of Yb atoms is about twice of that of Rb atoms, which will cause different gravitational sag in vertical orientation and leads to poor overlap. An optical dipole trap has to be designed to minimize the differential gravitational sag. In fact, two techniques have been presented and realized to alleviate gravitational sag between the clouds of two species^[24]. One can use a tight asymmetric trap to confine both species in the vertical direction. Besides, the elimination of the gravitational sag can be realized by adjusting the wavelength of one beam of crossed dipole trap^[25]. The SF-MI transition can be observed in the TOF image^[6,26] and excitation spectrum^[27], which

offer the methods to detect the MI state. Hence our proposal of the staggered MI is at the art of current experimental techniques.

In conclusion, a novel scheme for loading two species of atoms in a 3D optical lattice is presented. The most advantage of our scheme is that one can change the lattice depths for Rb and Yb atoms simultaneously by only varying the intensity of 532-nm laser. It is interesting that a staggered dual MI phase is predicted in this configuration of the optical lattice. The critical intensity of the phase transition is also predicted. The tunability of key parameters in our proposal opens up the new route to further investigate a variety of novel and interesting quantum phases in condensed-matter physics with the mixture of quantum degenerate gases.

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