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AUTHOR(S):
Kato, Shinya; Sugawa, Seiji; Shibata, Kosuke; Yamamoto, Ryuta; Takahashi, Yoshiro

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Control of Resonant Interaction between Electronic Ground and Excited States

Shinya Kato,1,* Seiji Sugawa,1 Kosuke Shibata,1 Ryuta Yamamoto,1 and Yoshiro Takahashi1,2
1Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
2JST, CREST, Chiyoda-ku, Tokyo 102-0075, Japan
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We observe magnetic Feshbach resonances in a collision between the ground and metastable states of two-electron atoms of ytterbium (Yb). We measure the on-site interaction of doubly occupied sites of an atomic Mott-insulator state in a three-dimensional optical lattice as a collisional frequency shift in a high-resolution laser spectroscopy. The observed spectra are well fitted by a simple theoretical formula, in which two particles with an s-wave contact interaction are confined in a harmonic trap. This analysis reveals a wide variation of the interaction with a resonance behavior around a magnetic field of about 1.1 G for the energetically lowest magnetic sublevel of 170Yb, as well as around 360 mG for the energetically highest magnetic sublevel of 174Yb. The observed Feshbach resonance can only be induced by an anisotropic interatomic interaction. This scheme will open the door to a variety of studies using two-electron atoms with tunable interaction.

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A microscopic property of a low energy binary collision determines a macroscopic behavior of an ultracold dilute atomic gas. Tuning the interaction between the atoms, one of the most fascinating aspects in this system, lies at the heart of recent numerous experimental progresses: the formation of ultracold molecules [1,2], a Bose-Einstein condensate (BEC) to a Bardeen-Cooper-Schrieffer (BCS) crossover with fermionic gases [3], Efimov trimer states [4,5], and so on [6]. So far, magnetically and optically tuned Feshbach resonances have been utilized [1,2], in which the interatomic interaction can be resonantly controlled through the coupling between an open channel and a closed channel.

Until now all the reported Feshbach resonances, magnetic or optical, were restricted to the collision between two electronically ground state atoms. In this Letter, we extend the possibility of the Feshbach resonance to the resonant control of the interaction between electronically excited and ground state atoms. We successfully observed magnetic Feshbach resonances in collisions between the ground 3S0 state and the metastable 3P2(mJ = ±2) states of two-electron atoms of ytterbium (Yb). Here mJ denotes the magnetic quantum number in the 3P2 state. See Fig. 1(a) for a schematic view of the energy levels of the colliding atoms in the lattice. The interatomic interaction is directly determined by a high-resolution laser spectroscopy of an atomic Mott-insulator state in a three-dimensional optical lattice with the ultranarrow optical 3S0 → 3P2 transition. A wide variation of the interaction with a resonance behavior is observed around a magnetic field of about 1.1 G for the energetically lowest magnetic sublevel mJ = −2 of 170Yb, as well as around 360 mG for the energetically highest magnetic sublevel mJ = +2 of 174Yb. It is noted that the unique feature of this 3S0 + 3P2 collision system is the anisotropy of the interaction which couples the different partial waves. In fact, this feature was well studied both experimentally and theoretically for various systems [7–15]. We have found that the observed variations of the scattering length can be consistently explained in terms of the anisotropic-interatomic-interaction-induced Feshbach resonance mechanism [16,17] and recently observed Feshbach resonances in Er are also connected to this mechanism [18]. Since the controlled collision between the long-lived metastable 3P state and the ground 3S0 state of the alkaline-earth-metal-like atoms has been explored as a useful platform for quantum computing and quantum simulation [19–22], our results provide a new possibility in such key applications.

Our experiment starts from a preparation of the ultracold 174Yb or 170Yb BEC, and the detailed procedure is

![FIG. 1 (color online).](image-url)

(a) Energy diagram of singly and doubly occupied sites in an optical lattice. The doubly occupied site has on-site energy shifts $U_{se}$ and $U_{ge}$ due to the interatomic interaction between two ground state atoms and between ground and excited state atoms, respectively. These energy shifts are revealed by a resonance shift of an excitation spectrum of the doubly occupied sites compared to that of the singly occupied sites. The interatomic potential between the atoms in the $3S_0$ and $3P_2$ states reflects the anisotropy interaction between them. (b) Relevant energy levels of a Yb atom for the spectroscopy.
with the above method for the

eous applications of two laser pulses which are resonant
suffer from the large inelastic collision rate between two
of the repumped atoms. It is noted that our method does
the MOT or the molasses is detected to measure the number
of the metastable $^3P_2$ and ground $^1S_0$ states. See Fig. 1(b)
for relevant energy levels. The detail of the procedure of
the spectroscopy is described in Ref. [23], and here we
briefly summarize the procedure. After the preparation of
the MOT, a portion of the ground state atoms is
directly excited to the $^3P_2$ state by a 0.25–1 ms laser pulse
whose wavelength is 507 nm. The atoms remaining in the
ground state are blasted out from the trap with a 0.2–0.3 ms
laser pulse which is resonant to the electric dipole allowed
$^1S_0 \leftrightarrow ^1P_1$ transition. The atoms in the excited state are
repumped to the ground state via the $^3S_1$ state by simulta-
nous applications of two laser pulses which are resonant to
the $^3P_2 \leftrightarrow ^3S_1$ and $^3P_0 \leftrightarrow ^3S_1$ transitions with the
duration of 0.5–1 ms. Finally, the repumped atoms are recap-
tured by a magneto-optical trap (MOT) with the $^1S_0 \leftrightarrow ^1P_1$
transition for $^{174}$Yb or by optical molasses with the
$^1S_0 \leftrightarrow ^1P_1$ transition for $^{170}$Yb. The fluorescence from
the MOT or the molasses is detected to measure the number
of the repumped atoms. It is noted that our method does not
suffer from the large inelastic collision rate between two
$^3P_2$ atoms, which was observed in Ref. [22]. The magnetic
field is determined from the spectroscopy of the $^1S_0 \leftrightarrow ^3P_2$
($m_J = +2$ and $-2$) transitions with the uncertainty of
about few mG.

In Fig. 2(a), we show the excitation spectra obtained
with the above method for the $^3P_2(m_J = +2)$ state of
$^{174}$Yb at various magnetic field strengths below 1 G. Note
that the frequency offset due to the Zeeman shift is
already subtracted in Fig. 2(a), and the zero frequency in
each spectrum corresponds to the resonance from the
singly occupied sites. The spectra show additional peaks
Corresponding to the resonances from the doubly and triply
occupied sites. The assignment of these peaks is confirmed
by the observations with different total number of atoms, in
which the peaks for multiply occupied sites only appear for
large enough number of atoms. In addition, the excitation
peaks to the higher vibrational state in the optical lattice
are observed around 28.5 kHz on the positive frequency
side in Fig. 2(a).

The interatomic interaction between the $^1S_0$ and $^3P_2$
states manifests itself in the spectrum as a filling-dependent
resonance frequency shift [24], as schematically depicted
in Fig. 1(a). In the following analysis of evaluating the
scattering length, we focus on the resonances from doubly
occupied sites which are indicated by arrows in Fig. 2(a).
In Fig. 2(b), the peak positions are plotted as a function of the
magnetic field. The resonance frequency shift between
the singly and doubly occupied sites is simply given by the
difference of the interatomic interaction between the
ground states $U_{gg}$ and that between the ground and excited
states $U_{ge}$. One can clearly see that the frequency separation
dramatically changes when the magnetic field strength
changes. This behavior directly indicates the change of
the interatomic interaction with a magnetic field. Here the
interatomic interaction between the ground states $U_{gg}$ is
described as

FIG. 2 (color online). (a) Excitation spectra for $^3P_2(m_J = +2)$
state of $^{174}$Yb at various magnetic field strengths below 1 G. The
insets show enlarged views of low frequency side of the corre-
sponding spectra. The arrows indicate the resonances from the
doubly occupied sites. The Zeeman shift in each spectrum is
subtracted and the spectra are shifted vertically for clarity. The
solid lines denote the fits with Gaussian functions for each of
the resonances (see text). Plots of resonance peak positions (b) as a
function of a magnetic field and (c) as a function of a scattering
length $a_{sc}$ evaluated by using the analytic formula Eq. (2). Here
$a_0$ is the Bohr radius. The rectangles denote the resonances for
the singly occupied sites and excitations to the higher
vibrational state, and the circles for the doubly occupied sites. The
analytical curve based on Eq. (2) is indicated by the solid line, and zero
and the trap frequency are indicated by the dashed lines. The error bars
in (b) and (c) represent the standard error of the Gaussian fits.
(d) Evaluated scattering length $a_{sc}$ as a function of a magnetic
field. The solid line denotes a fit with a function $a_{sc}(B) = a_{bg} - (a_{bg} \Delta)/(B - B_0)$, with $a_{bg} = -3.4 \pm 2.5$ nm, $\Delta = 2.3 \pm 1.6$ G,
and $B_0 = 360 \pm 10$ mG.
dependence of the evaluated scattering length $a_{ge}$ on $U_{gg}$, we utilize a theoretical formula given in Ref. [26] where two particles with a contact interaction are confined in an isotropic harmonic trap. This is important because we cannot use a simple formula like Eq. (1) when the scattering length becomes close to the harmonic oscillator length $a_{HO} = \sqrt{\hbar/(m\omega)}$. Here $m$ is the mass of the atom and $\omega$ is the mean trap frequency. The interatomic interaction $U_{gg}$ is related to the scattering length $a_{ge}$ by the following analytical formula [27]:

$$
a_{HO}/a_{ge} = \sqrt{2} \frac{\Gamma(-U_{ge}/(2\hbar\omega) + 3/4)}{\Gamma(-U_{ge}/(2\hbar\omega) + 1/4)},$$

(2)

where $\Gamma(x)$ is the Gamma function.

The results of the analysis are shown in Fig. 2(c) where the resonance peak positions are plotted as a function of the evaluated scattering length $a_{ge}$ as well as the energy spectrum calculated from Eq. (2). In the analysis of the data for the magnetic field up to 490 mG, we use the resonance frequencies corresponding to the doubly occupied sites in the negative frequency side in Fig. 2(a), since the peaks in the positive frequency side are overlapped with the closely located blue sidebands. For the magnetic field larger than 490 mG, the resonance frequencies in the positive frequency side are overlapped with the closely located blue sidebands. In order to evaluate the scattering length $a_{ge}$, we similarly evaluate the scattering length $a_{ge}$ of $\text{Sr}$. Note that $a_{ge}$ equals 3.38 nm for $\text{Sr}$ [25], the observed variation of the resonance peak positions is attributed to the variation of $U_{gg}$.

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It is noted that the matrix element of Eq. (4) has a nonzero value for \( \Delta l = l' - l = 2 \). Figure 4(a) shows the relevant energy levels. Magnetic sublevels of \( m_J > -2 \) with the higher partial wave \( l = 2 \) can in general form a bound state inside the centrifugal barrier, as schematically shown by a horizontal solid line in Fig. 4(a). Among many states, that with \( (m_J, m_l) = (-1, -1) \) or \( (0, -2) \) can have a total magnetic quantum number \( M = -2 \), and thus can be coupled with the open channel, which results in the Feshbach resonance. Therefore, the observed variation of the scattering length can be consistently explained in terms of the anisotropy-induced Feshbach resonance. Note that the \( 3P_2(m_J = -2) \) state does not suffer from the Zeeman-sublevel changing collision, and thus it is encouraging to use this Feshbach resonance for controlled collision in a variety of proposed applications in quantum computation and quantum simulation.

In the case of \(^{170}\text{Yb}\), the resonant variation of the scattering length is observed for the \( 3P_2(m_J = +2) \) state which is energetically highest among the Zeeman sublevels of \( 3P_2 \). At first glance, this is surprising because all the Feshbach resonances previously observed have closed (resonance) channels which are energetically higher than the open channel at a long internuclear distance, and such channels are absent in the present case. We can, however, provide an explanation of this phenomenon by a combination of the anisotropy-induced Feshbach resonance and a shape resonance [28]. The \(^1S_0\) + \(^3P_2\) interatomic interaction along with the centrifugal potential barrier associated with a higher partial wave can form a bound state within the potential barrier above the dissociation threshold, which is known as a shape resonance. A possible energy level of the shape resonance is schematically depicted as the horizontal solid line in Fig. 4(b). When we consider a shape resonance for lower magnetic sublevels \( m_J < +2 \), it is not surprising that the energy of such a bound state can be close to or higher than that of the open channel of \( m_J = +2 \), which is set to zero in Fig. 4(b). Note that the observed magnetic field dependence of the scattering length is consistent with this scenario: due to the lower magnetic moment of the closed channel compared with the open channel, the energy of the closed channel can be lower than that of the open channel at a high-field side of the resonance, and can be higher at a low-field side.

In conclusion, we observe the magnetically tuned interatomic interaction between different electronic orbitals through the high-resolution laser spectroscopy of the Mott insulator in the 3D optical lattice. The experimental observations are analyzed by the analytical solution of interacting two atoms in the harmonic trap. The evaluated scattering length shows a resonant variation around the magnetic field of about 1.1 G for \( m_J = -2 \) of \(^{170}\text{Yb}\), as well as around 360 mG for \( m_J = +2 \) of \(^{174}\text{Yb}\). In the present system, an anisotropic electronic interaction [11,29] can induce a Feshbach resonance between different partial waves [16,17]. Since several closed channels with different angular momentum can participate in the coupling to an open channel in the anisotropy-induced Feshbach resonance, we can expect many resonances as in the cases of Er [18] and Dy [16,17]. A further theoretical calculation is quite helpful to obtain full quantitative explanation of the observed phenomena, including the position and width of the resonances as well as the identification of the magnetic quantum number corresponding to the closed channel.

Our work will open the door to a variety of studies using two-electron atoms with tunable interaction, especially quantum computing and quantum simulation [19–22] in which the controlled collision between the metastable \(^3P\) state and the ground \(^1S_0\) state is a key ingredient. The anisotropy-induced Feshbach resonances are also expected for other isotopes. An especially interesting case is the fermionic isotopes of \(^{171}\text{Yb}\) and \(^{173}\text{Yb}\), where the spin-polarized sample in the \(^3P\) state will not suffer from the inelastic collision [22,30] owing to the Pauli exclusion, and we can possibly study BCS pairing of ground and metastable states. In addition, we can also expect similar Feshbach resonances for a mixture system of the ground state of alkali-metal atoms and the metastable state of alkali-earth-metal atoms. This possibility is especially important since the magnetic Feshbach resonance between the ground states of alkali-metal atoms and alkali-earth-metal atoms is, although it exists, mostly very narrow and located at high magnetic fields [31,32].

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*shinya_k@scphys.kyoto-u.ac.jp

[27] It is noted that the trap frequencies for the $^1S_0$ state and the $^3P_2(m_J = \pm 2)$ state are $2\pi \times 26.5$ kHz and $2\pi \times 28.5$ kHz, respectively, and not the same in general due to the different polarizability for these states at the wavelength of the optical trap and optical lattice. Though the difference between the trap frequencies causes the mixing of the center-of-mass motion and relative motion, this mixing effect to the eigenenergy is negligible within the first-order perturbation. Therefore, we use this model without considering the mixing effect and adopt the average of these two trap frequencies for the calculation.
[29] P. Zhang and T. V. Tscherbul (private communication).