
Optical lattice quantum simulation of multi-body force and nonequilibrium dynamics in isolated and open systems

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ABSTRACT

Now, more than 40 years after the proposal of quantum simulation by R. P. Feynman, we are witnessing remarkable progress in artificial quantum systems, which serve as ideal platforms for quantum simulation. In particular, ultracold atoms in an optical lattice have offered a versatile playground with high and rich controllability, allowing the study of a wide variety of systems, from quantum few-body systems to quantum many-body systems. In this thesis, we present three quantum simulation experiments in optical lattice systems: multi-body force and nonequilibrium dynamics in isolated and open systems.

First, we report an experimental study of a few-body bosonic atom system in a strongly interacting regime beyond the perturbative treatment of the bare two-body interaction in previous works. This becomes possible by precisely controlling the two-body interaction via a Feshbach resonance, combined with a high-resolution inter-orbital clock spectroscopy. As an important illustration of entering a strongly interacting regime, we find an interesting feature of the effective three-body interactions in comparison with the perturbation calculation. Furthermore, we obtain a clear signature of an effective four-body interaction, evidenced by the binding energies of four or more atoms in a lattice site.

Second, we report an experimental study of a dissipative Fermi-Hubbard system with on-site two-body losses, which is introduced in a controlled manner utilizing a photoassociation technique. Here, by directly measuring the spin correlation dynamics between nearest-neighbor sites, we successfully observe the sign reversal of the magnetic correlation from antiferromagnetic to ferromagnetic in double wells. We systematically measure the spin correlation dynamics in an isolated double-well optical lattice, as well as a crossover from an isolated double-well lattice to a one-dimensional uniform lattice. In a wide range of lattice configurations over an isolated double-well lattice, we observe a ferromagnetic spin correlation, which is consistent with a Dicke type of correlation expected in the long-time limit.

Third, we report an experimental study of the one-dimensional Bose-Hubbard system with neither disorder nor tilt potential, which has been predicted to exhibit Hilbert-space fragmentation (HSF) caused by a strong interatomic interaction. Specifically, we analyze far-from-equilibrium dynamics starting from a period-two charge-density wave of doublons with a small portion of singlons in a singlon and doublon-resolved manner to reveal a slowing-down of the relaxation in a strongly interacting regime. Importantly, we find that the numbers of singlons and doublons are conserved during the dynamics, indicating HSF as a mechanism of the observed slow relaxation. Furthermore, we also reveal the role of

doublon-singlon interactions in the dynamics.

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INTRODUCTION

1.1 Quantum simulation with ultracold atoms in an optical lattice

In 1981, R. P. Feynman proposed the concept of quantum simulation in his seminal lecture titled "Simulating physics with computers", concluding with the statement "*..., because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, ...*" [1]. Quantum simulation means to simulate a quantum system of interest with another highly controllable quantum system, which is called a quantum simulator. Here, there are two types of quantum simulators: an analog one, which simulates a specific type of Hamiltonian, and a digital one, which performs universal quantum simulation by discrete quantum-gate operations. By mapping theoretical models, which often model real materials and are difficult to calculate exactly due to the exponential growth of computational costs with the size of quantum systems, to quantum simulators and simulating the models, we endeavor to obtain new insights and understandings to them [2, 3, 4].

Now, more than 40 years after that proposal and one hundred years after the birth of quantum mechanics, we are witnessing remarkable progress in artificial quantum systems; Quantum systems are no longer objects to be merely observed, and they are objects to be actively controlled. Here, ultracold gases in optical lattices [5, 6, 7, 8, 9] and optical tweezer arrays [10, 11], trapped ions [12, 13], superconducting qubits [14], photonic quantum system [15], etc., serve as examples of such systems and have been ideal platforms especially for analog quantum simulation. For these systems, we also see today's fierce competition to implement fault-tolerant quantum computation beyond noisy intermediate-scale quantum computation [16, 17, 18, 19].

Among them, ultracold gases have gained widespread attention since the first experimental realization of quantum degenerate bosonic gases, Bose-Einstein condensates, in 1995 [20, 21, 22], soon followed by the realization of Fermi degenerate gases [23, 24]. In particular, ultracold atoms in an optical lattice, which is a periodic potential created by interfering counter-propagating laser beams, have been utilized considerably to study a wide variety of systems, from quantum few-body systems to quantum many-body systems (Fig. 1.1).

This optical lattice system is a clean system in which there are no lattice defects or impurities. Moreover, the optical lattice system is a programmable system in the sense that it has high and rich controllability over various system parameters: not only the potential depth of the lattice, atom filling in a lattice, and temperature of the system, but also the lattice geometry and dimensionality of the system, and quantum statistics (bosonic, fermionic, and also these mixed systems) can be controlled. Furthermore, the celebrated Hubbard model [25, 26], which describes the strongly correlated quantum many-body systems and lies at the heart of condensed matter physics, can be realized in the optical lattice system [27, 28]. Therefore, along with the high controllability over parameters in the Hubbard model, such as tunneling amplitudes between sites and on-site interaction strengths, the optical lattice system has served as an analog quantum simulator, or optical lattice quantum simulator, for elucidating complex behaviors of strongly correlated quantum many-body systems.

A milestone experiment in the optical lattice system is the observation of a quantum phase transition from a superfluid to a Mott insulator in the Bose-Hubbard system [29], and also a direct imaging of Fermi surfaces in the Fermi-Hubbard system [30]. The main advantages of an optical lattice quantum simulator include its high scalability, the ability to trace quantum dynamics easily in a real-time manner, and the availability of various measurement methods, such as time-of-flight measurement, band-mapping technique, and spectroscopic techniques. Also, a quantum gas microscope (QGM) has been a quite powerful tool in the optical lattice system [31, 32]. This tool allows us to observe the local density distribution of atoms in an optical lattice at single-site resolution. A QGM has paved the way toward a deeper understanding of strongly correlated quantum many-body systems, as exemplified by the observation of a many-body localization transition in a disordered two-dimensional system [33] and the observation of long-range antiferromagnetic order in the Fermi-Hubbard system [34]. Also, it has expanded the possibilities of the optical lattice experiment, as exemplified by the measurement of entanglement entropy in a quantum many-body system [35].

During my PhD course, I performed three quantum simulation experiments using optical lattice systems, making great use of its advantages. The first is a study of the effective multi-body interaction in a quantum few-body system, which is realized in each optical lattice site. The second is a study of nonequilibrium dynamics of quantum magnetism in an open system, where dissipation, an on-site two-body loss, is introduced. The third is a study of nonequilibrium dynamics in an isolated system, or quantum thermalization in an isolated system, starting from a sudden quench of the optical lattice depth. In the following,

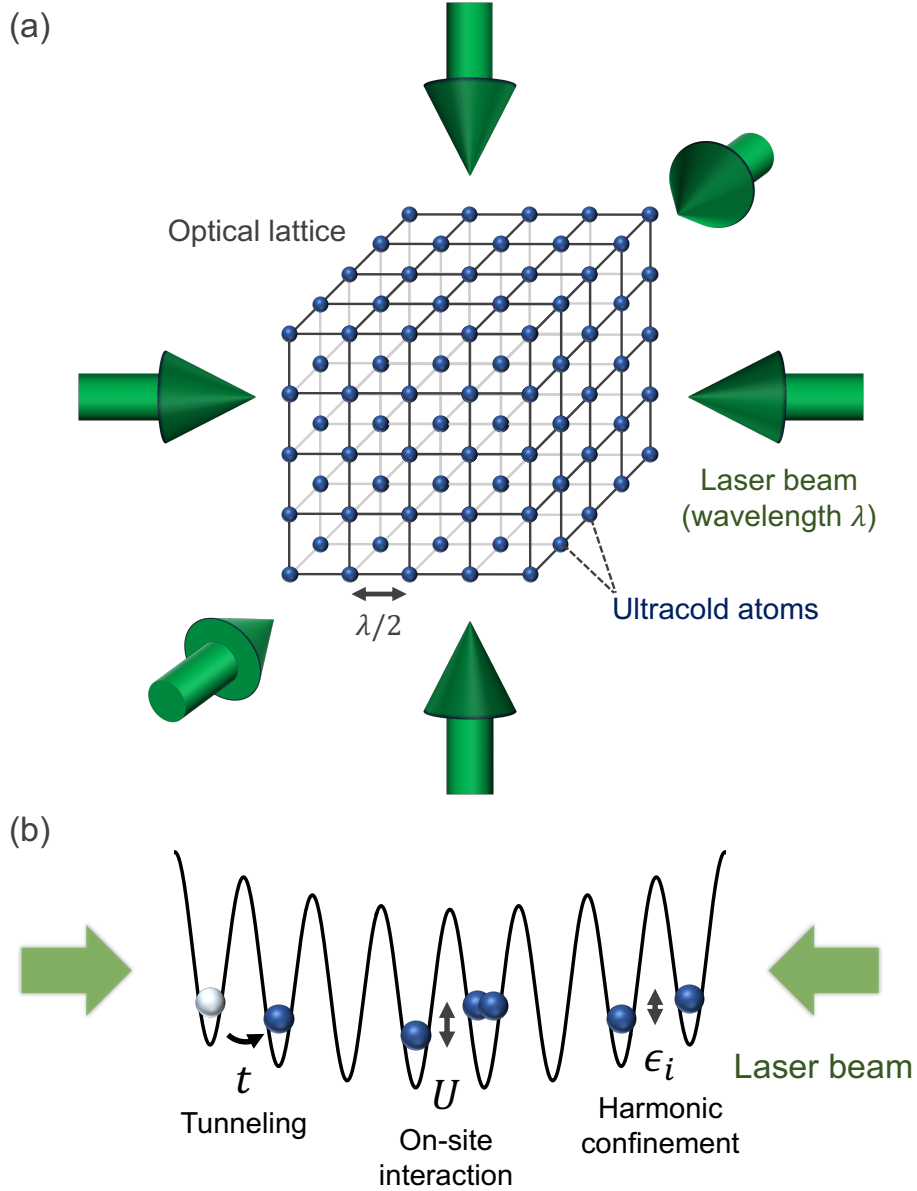


Figure 1.1: Schematic of an optical lattice. (a) Three-dimensional cubic optical lattice formed by superimposing three orthogonal standing waves, which are generated by counter-propagating laser beams. (b) Ultracold atoms trapped in an optical lattice potential. The dynamics of this system is well described by the Hubbard model, which consists of the tunneling t , the on-site interaction U , and the harmonic confinement ϵ_i .

we briefly introduce each of these topics.

1.2 Effective multi-body interaction in a quantum few-body system

A few-body quantum system is usually defined as one that consists of a small number of well-defined constituent particles, often trapped or self-trapped under some confining potential [36]. Few-quark states, light nuclear and hadronic systems, few-electron atomic and molecular systems, quantum dots, and trapped cold-atom systems are the typical examples and have recently been studied extensively and intensively [37, 38, 39]. In these few-body systems, a two-body interaction or force between constituent quantum particles, usually described by scattering lengths at low collision energy, plays a dominant role in the quantitative description of the system.

In nuclear physics, for instance, the details of the two-body nucleon-nucleon interaction via one-boson exchange potential are now rather well established [40, 41, 42]. Several important observations, however, cannot be explained in terms of the simple pairwise interaction, and the effective three-body force between nucleons has been introduced to resolve the discrepancies. Illustrative examples involve the binding energies of light nuclei like triton (${}^3\text{H}$) [43, 44] and ${}^{3,6,8}\text{He}$ [45], the deuteron-nucleon scattering cross section [46, 47, 48, 49], the equation of state of nuclear matters like a massive neutron star [50] and the anomaly on the limit of neutron-rich nuclei, namely the neutron drip line [51]. Here, the most well-known microscopic mechanism of the effective three-body force is known as the Fujita-Miyazawa type [52], which is induced by the virtual Δ excitations via the two-body nuclear force due to pion exchange.

Ultracold atoms have also provided a useful platform for studying few-body atomic systems. For example, a novel phenomenon of the Efimov effect is investigated, where an effective three-body interaction emerges via multiple scatterings via resonant two-body interactions, resulting in a series of universal weakly-bound states characterized by a three-body parameter. Similarly, four- and more atom-bound states are observed and explained by using a three-body parameter or potential [53, 54]. Another important example of a few-body atomic system is a well-localized few-atom system tightly confined in each of an optical lattice potential, and the effective three-body interaction has been extensively studied with various methods such as quantum phase collapse and revival technique [55], lattice modulation spectroscopy [56], high-resolution clock spectroscopy both for bosons [57, 58, 59] and fermions [60], and the results are quantitatively explained by perturbative calculations [61, 62, 63].

The procedure of determining the energies with the perturbation theory is elaborated on in Ref. [62]. The emergence of the effective interaction is understood in the physical picture based on the microscopic description by integrating out the degrees of freedom of virtual excitations to higher vibrational states. Here, we can find an analogy with the effec-

tive three-body force of Fujita-Miyazawa type in nuclear physics, where nucleons, a bare two-body nuclear force, and the Δ excitations correspond to the atoms in the vibrational ground state of a harmonic trap, the bare two-body interatomic force, and the vibrational excitations of the atoms, respectively.

A few-body quantum system in a strongly-interacting regime beyond the perturbation is, in general, by no means trivial. Note that, already discussed in a pioneering theoretical work [64], the strong interaction of the two-body system appears as the nonlinearity of the interaction energy with respect to the scattering length a_s when a_s is comparable to or larger than the confining harmonic oscillator length, and was observed experimentally (see e.g. [6] and also [58, 65, 66]). In contrast, beyond a two-body problem, a few-body quantum system in a strongly-interacting regime has not been assessed, and revealing the behavior will give insights into the nuclear systems where the non-perturbative treatments are generally quite difficult.

1.3 Quantum magnetism in dissipative quantum systems

Dissipation, which is caused by the coupling to the surrounding environment and exemplified by particle loss and photon scattering, plays a crucial role in quantum systems. On the one hand, it disturbs the coherent dynamics in quantum systems, which is unfavorable for many quantum information processing as well as the study of quantum phases. On the other hand, dissipation can play a novel role in preparing and manipulating quantum states of interest [67, 68, 69]. In cold atom and molecule systems, which are often regarded as ideal isolated quantum systems, it is also possible to study open quantum systems by making use of their high controllability. So far, dissipative atomic and molecular systems with one- [70, 71, 72, 73, 74, 75], two- [76, 77, 78, 79, 80], and three-body particle losses [81, 82, 83] have been investigated, where, one-, two-, and three-body losses are implemented by a tight electron beam or photon scattering, an inelastic collision between particles in a particular state or between particles via photoassociation (PA), and three-body recombination by a Feshbach resonance, respectively. By those studies, part of the novel phenomena brought about only by the presence of dissipation has been clarified.

In quantum magnetism, which is a many-body state of spins and emerges owing to effective spin-spin interactions mediated by the virtual exchange of particles in a Mott insulator, dissipation can also have a great influence on its equilibrium state. In the previous work, especially in Ref. [84], sign reversal of magnetic correlations in dissipative Hubbard models with on-site two-body losses is theoretically predicted; Antiferromagnetic correlation change to ferromagnetic one in a fermionic Mott insulator, and ferromagnetic correlation change to antiferromagnetic one in a bosonic Mott insulator in the presence of an inelastic Hubbard interaction. For a dissipative system, the formation of a highly entangled Dicke state [85], which has a fully symmetric spin wave function, is also predicted [86, 87]. Experimentally, atom loss dynamics in the one-dimensional (1D) dissipative Fermi-Hubbard system has been investigated, and the dynamical generation of the Dicke

state has been inferred based on the suppressed atom losses after initial fast transient dynamics [88]. However, in Ref. [88], spin correlations, which are a more direct signature of the ferromagnetism characterizing the Dicke state, have not been measured. Moreover, a fixed strength of dissipation was introduced, and therefore, a systematic study of dissipative dynamics with controllable strength of dissipation was not carried out.

1.4 Thermalization in quantum many-body systems

The problem of quantum thermalization, i.e., how isolated quantum many-body systems that undergo the reversible unitary time evolution can reach thermal equilibrium states, lies at the heart of modern quantum statistical physics and is of considerable recent interest. As a mechanism of the thermalization, the eigenstate thermalization hypothesis (ETH) is known, which states that expectation values of physical quantities for eigenstates of a quantum many-body system coincide with that of the microcanonical ensemble in the corresponding energy [89, 90, 91, 92]. Especially, when a quantum many-body system satisfies the strong version of the ETH, where all of the eigenstates satisfy the ETH, the long-time average of the physical quantity coincides with the microcanonical average, that is, the system thermalizes [93, 94].

The artificial quantum systems, mentioned in the first section, have enabled indispensable studies of thermalization, both experimentally and theoretically. To better understand the mechanisms of thermalization, the investigation of nonergodic systems, which do not show thermalization, is important. Illustrative examples of nonergodic systems include integrable [95, 96, 97, 98, 99, 100] and many-body localized (MBL) systems [101, 102, 103, 104, 105, 106, 33, 107, 108, 109, 110, 111, 112], where thermalization is prevented due to the presence of an extensive number of conserved quantities and the strong disorder potential, respectively. Furthermore, the recent findings of another type of nonergodic systems show the diversity of origins of nonergodic behavior, as exemplified by quantum many-body scar [113, 114, 115, 116, 117, 118, 119, 120, 121, 122], Stark MBL [123, 124, 125, 126] and Hilbert-space fragmentation (HSF) [127, 128, 129, 130, 131, 132, 133, 134].

In particular, HSF typically results from the presence of nontrivial conserved quantities, leading to strong kinetic constraints on the system. Under such constraints, the Hilbert space is fragmented into an exponentially large number of disconnected subsectors (Krylov subsectors), and the dynamics are restricted to only a few subsectors, preventing the system from thermalizing. Experimentally, the nonergodic dynamics due to the HSF have been observed, especially in the 1D Fermi-Hubbard system [129, 130] and the two-dimensional Bose-Hubbard system [134], where linear potential gradients (tilt potentials) are applied, and the total atom number and dipole moment are conserved. Theoretically, a disorder-free 1D Bose-Hubbard model with no trapping potential [135, 136] and with a trapping potential [137, 138, 124] has been studied. Especially in Ref. [138], it has been reported that the nonergodic behavior emerges in the strongly interacting regime when the dynamics start from a period-two charge-density wave (CDW) of doublons (atoms in doubly occu-

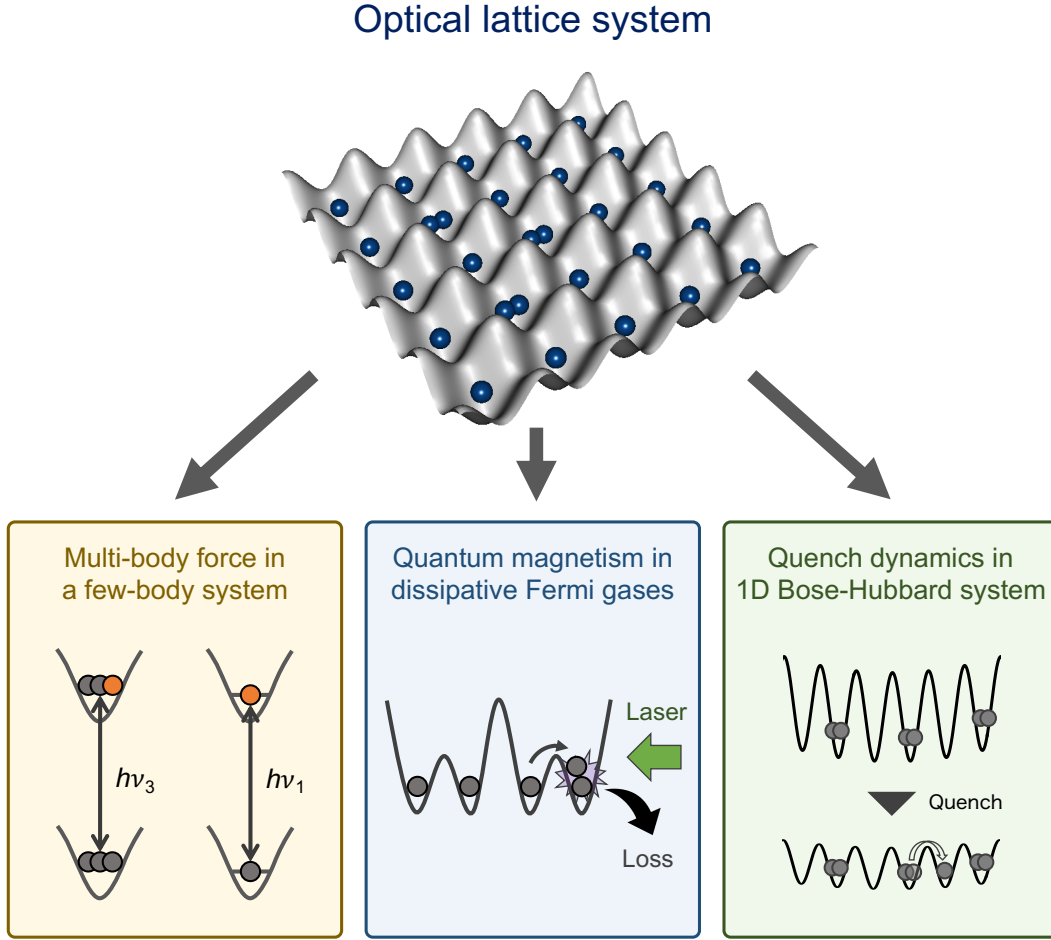


Figure 1.2: Schematic of our works.

pied sites), while rapid relaxation occurs starting from that of singlons. In this system, in addition to the total atom number, the numbers of doublons and singlons are emergent conserved quantities in the strongly interacting regime, which gives rise to HSF.

1.5 This thesis

In this thesis, we present three quantum simulation experiments on the above three topics using optical lattice systems (Fig. 1.2).

First, we report an experimental study of a few-body bosonic atom system in a strongly interacting regime beyond the perturbative treatment of the bare two-body interaction in previous works. This becomes possible by precisely controlling the two-body interaction via a Feshbach resonance, combined with a high-resolution inter-orbital clock spec-

troscopy. As an important illustration of entering a strongly interacting regime, we find an interesting feature of the effective three-body interactions in comparison with the perturbation calculation. Furthermore, we obtain a clear signature of an effective four-body interaction, evidenced by the binding energies of four or more atoms in a lattice site. Our results not only provide new insights into few-body quantum systems but also serve as a valuable and precise benchmark for theoretical approaches to them in a strongly interacting regime well beyond the regime where the perturbation theory applies.

Second, we report an experimental study of a dissipative Fermi-Hubbard system with on-site two-body losses, which is introduced in a controlled manner utilizing a PA technique. Here, by directly measuring the spin correlation dynamics between nearest-neighbor sites, we successfully observe the sign reversal of the magnetic correlation from antiferromagnetic to ferromagnetic in double wells. We systematically measure the spin correlation dynamics in an isolated double-well optical lattice, as well as a crossover from an isolated double-well lattice to a one-dimensional uniform lattice. In a wide range of lattice configurations over an isolated double-well lattice, we observe a ferromagnetic spin correlation, which is consistent with a Dicke type of correlation expected in the long-time limit. This work is valuable as a demonstration of the control of quantum magnetism in open quantum systems with dissipation.

Third, we report an experimental study of the one-dimensional Bose-Hubbard system with neither disorder nor tilt potential, which has been predicted to exhibit HSF caused by a strong interatomic interaction. Specifically, we analyze far-from-equilibrium dynamics starting from a period-two CDW of doublons with a small portion of singlons in a singlon and doublon-resolved manner to reveal a slowing-down of the relaxation in a strongly interacting regime. Importantly, we find that the numbers of singlons and doublons are conserved during the dynamics, indicating HSF as a mechanism of the observed slow relaxation and providing the first experimental confirmation of the conserved quantities responsible for HSF. Furthermore, we also reveal the role of doublon-singlon interactions in the dynamics, which offers important insights into the quantum thermalization dynamics. This work is expected to deepen our understanding of the non-thermalizing behaviors due to HSF.

Outline of this thesis

This thesis is organized as follows.

- Chapter 2 introduces theoretical backgrounds for the quantum simulation experiment in an optical lattice.
- Chapter 3 introduces the details of our experimental setup and experimental techniques related to this work.
- Chapter 4 describes the study of the effective multi-body interaction in a strongly interacting regime in a trapped ultracold atom system.

- Chapter 5 describes the study of quantum magnetism in a dissipative Fermi gas with on-site two-body losses.
- Chapter 6 describes the study of the nonequilibrium dynamics following the sudden quench of the optical-lattice depth in strongly interacting Bose-Hubbard chains.
- Chapter 7 briefly reviews the achievements in each work presented in this thesis and presents some future outlooks on them.

THEORETICAL BACKGROUND

In this chapter, we introduce the theoretical backgrounds for optical lattice experiments. First, we briefly summarize thermodynamic quantities for the ideal Bose and Fermi gases in a three-dimensional (3D) harmonic trap. Then, in Sec. 2.2, we describe a band structure in an optical lattice and an optical superlattice, and introduce the Bose-Hubbard and Fermi-Hubbard models.

2.1 Ideal gases in a harmonic trap

In this section, we describe the ideal Bose gases and Fermi gases in a 3D harmonic trap and derive the expression of thermodynamic quantities for each gas [139, 140, 141]. Note that ultracold gases are generally dilute and can be treated as ideal (non-interacting) gases. For example, in the case of Fermi gases, a dimensionless parameter $k_F a_s$ represents the ratio of the interatomic interaction energy to the kinetic energy of atoms, where $k_F = (6\pi^2 n_\sigma)^{1/3}$ and a_s are the Fermi wave number for an atomic density n_σ for each spin state σ and the s -wave scattering length, respectively. In a typical experimental condition, the dimensionless parameter $k_F a_s$ is about a few percent for $n_\sigma = 10^{-13} \text{ cm}^{-3}$ and a_s of few nanometers, so we can regard ultracold Fermi gases as ideal gases. Also, in the case of Bose gases, a dimensionless parameter $n_\sigma a^3 \ll 1$ (equivalent to $k_F a_s \ll 1$ in the Fermi gas case) is satisfied for non-condensed atoms (thermal atoms), so we can regard non-condensed Bose gases as ideal gases.

We first introduce the density of single-particle states for ideal gases in a 3D harmonic trap. The density of states is defined under the semi-classical approximation as follows:

$$D(E) = \mathcal{N} \int \frac{d\mathbf{r} d\mathbf{p}}{(2\pi\hbar)^3} \delta(E - E(\mathbf{r}, \mathbf{p})), \quad (2.1)$$

where $E(\mathbf{r}, \mathbf{p}) = \mathbf{p}^2/2m + V_{\text{ext}}(\mathbf{r})$; $V_{\text{ext}}(\mathbf{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$ is a 3D harmonic trap potential, where ω_i ($i = x, y, z$) is a trap frequency and $\mathcal{N}$ is the spin degrees of freedom. Here, the semi-classical approximation is valid when the temperature of the atomic gas T is much larger than the single-particle energy level spacing $\hbar\bar{\omega}$, i.e., $k_B T \gg \hbar\bar{\omega}$, where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of trap frequencies, and which is satisfied in a typical experimental condition. By calculating Eq. (2.1), we obtain the density of states for a single particle in a 3D harmonic trap as follows:

$$D(E) = \mathcal{N} C_3 E^2, \quad (2.2)$$

where $C_3 = 1/(2(\hbar\bar{\omega})^3)$. Below, we calculate thermodynamic quantities for ideal Bose gases and Fermi gases.

2.1.1 Ideal Bose gases

When the temperature of an atomic gas T is below T_c , where T_c is the critical temperature for Bose-Einstein condensation, the atom number in excited states (thermal component atoms) is given as follows (below we set $\mathcal{N} = 1$):

$$\begin{aligned} N_{\text{ex}} &= \int_0^\infty dE D(E) \bar{n}(E) \\ &= C_3 \Gamma(3) \zeta(3) (k_B T)^3, \end{aligned} \quad (2.3)$$

where $\bar{n}(E) = 1/(\exp(E/k_B T) - 1)$ is the Bose distribution function (the average particle occupation number for the energy E) with the chemical potential $\mu = 0$, where k_B is the Boltzmann constant; $\Gamma(\alpha)$ is the gamma function; and $\zeta(\alpha) = \sum_{n=1}^\infty n^{-\alpha}$ is the Riemann zeta function. Here, the critical temperature T_c is determined by the condition $N_{\text{ex}}(T = T_c, \mu = 0) = N$, where N is the total atom number in the system, and given as follows:

$$k_B T_c = \frac{N^{1/3}}{[C_3 \Gamma(3) \zeta(3)]^{1/3}} = \hbar\bar{\omega} \frac{N^{1/3}}{[\zeta(3)]^{1/3}}, \quad (2.4)$$

where we have used $\Gamma(3) = 2$. Using Eqs. (2.3) and (2.4), we obtain the condensed atom fraction as follows:

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c} \right)^3, \quad (2.5)$$

where N_0 is the condensed atom number.

Next, we calculate the internal energy below T_c , where only excited states contribute to the total energy, as follows:

$$\begin{aligned} E_{\text{tot}} &= \int_0^\infty dE D(E) \bar{n}(E) E \\ &= C_3 \Gamma(4) \zeta(4) (k_B T)^4 = 3N k_B \frac{\zeta(4)}{\zeta(3)} \frac{T^4}{T_c^3}, \end{aligned} \quad (2.6)$$

where we have used a property of the gamma function that $\Gamma(\alpha+1) = \alpha\Gamma(\alpha)$. Using Eq. (2.6), we obtain the expression of the specific heat C , which is given by $C = \partial E / \partial T$, as follows:

$$C = 12Nk_B \frac{\zeta(4)}{\zeta(3)} \left(\frac{T}{T_c} \right)^3. \quad (2.7)$$

Also, we obtain the expression of the entropy S , which is given by $S = \int dT C/T$, as follows:

$$S = 4Nk_B \frac{\zeta(4)}{\zeta(3)} \left(\frac{T}{T_c} \right)^3. \quad (2.8)$$

2.1.2 Ideal Fermi gases

Considering non-interacting Fermi gases of the total atom number N , this satisfies the following condition:

$$N = \int_0^{E_F} dE D(E), \quad (2.9)$$

where E_F is the Fermi energy and determined by this equation as follows:

$$E_F = \left(\frac{6N}{\mathcal{N}} \right)^{1/3} \hbar\bar{\omega}. \quad (2.10)$$

Also, the Fermi temperature T_F is defined as $T_F = E_F / k_B$, and T_F is on the order of 100 nK in typical experimental conditions. Here, the temperature normalized by the Fermi temperature T_F , i.e., T/T_F , is a measure of the degree of quantum degeneracy of a Fermi gas.

Below, we deal with an ideal Fermi gas as a ground canonical ensemble to derive the expression of thermodynamic quantities. The ground partition function Z is given as follows:

$$Z = \int_0^\infty dE D(E) \left(1 + e^{-(E-\mu)/k_B T} \right). \quad (2.11)$$

Using Eq. (2.11), we obtain the following ground potential $\Omega(T, \mu)$:

$$\begin{aligned} \Omega(T, \mu) &= -k_B T \ln(Z) = -k_B T \int_0^\infty dE D(E) \ln \left(1 + e^{-(E-\mu)/k_B T} \right) \\ &= \frac{\mathcal{N}(k_B T)^4}{(\hbar\bar{\omega})^3} \text{Li}_4(-z), \end{aligned} \quad (2.12)$$

where $z = e^{\mu/k_B T}$ is the fugacity; and $\text{Li}_\alpha(z)$ is the Polylogarithmic function defined as follows:

$$\text{Li}_\alpha(-z) := -\frac{1}{\Gamma(\alpha)} \int_0^\infty dx \frac{x^{\alpha-1}}{z^{-1}e^x + 1} = \sum_{k=1}^\infty \frac{(-z)^k}{k^\alpha}, \quad (2.13)$$

where $\Gamma(\alpha)$ is the gamma function, and this satisfies $\Gamma(\alpha) = (\alpha-1)!$ when $\alpha \in \mathbb{N}$. Using Eq. (2.12), we obtain the expressions of the total atom number N and the entropy S as follows:

$$\left\{ \begin{array}{l} N = -\frac{\partial \Omega}{\partial \mu} = -\mathcal{N} \left(\frac{k_B T}{\hbar\bar{\omega}} \right)^3 \text{Li}_3(-z), \end{array} \right. \quad (2.14)$$

$$\left\{ \begin{array}{l} S = -\frac{\partial \Omega}{\partial T} = Nk_B \left(4 \frac{\text{Li}_4(-z)}{\text{Li}_3(-z)} - \ln z \right), \end{array} \right. \quad (2.15)$$

where we have used a property of the Polylogarithmic function that $d\text{Li}_\alpha(z)/dz = \text{Li}_{\alpha-1}(z)/z$. From Eqs. (2.10) and (2.14), we obtain the following equation for T/T_F :

$$\frac{T}{T_F} = \left(-\frac{1}{6\text{Li}_3(-z)} \right)^{1/3}. \quad (2.16)$$

2.2 Ultracold atoms in an optical lattice

In this section, we first describe the eigenvalue problem of a single particle in a general periodic potential. Then, in Sec. 2.2.2 and Sec. 2.2.3, we introduce a band structure of a monochromatic optical lattice and an optical superlattice, respectively. In Sec. 2.2.4, we describe the Hubbard parameters for a monochromatic optical lattice and an optical superlattice.

2.2.1 Single particle in a general periodic potential

We consider a single particle in a general one-dimensional (1D) periodic potential $V(x)$. The Hamiltonian for this system is given as follows:

$$H = H_0 + V(\hat{x}) = \frac{\hbar^2 \hat{k}^2}{2M} + V(\hat{x}), \quad (2.17)$$

$$V(\hat{x} + d) = V(\hat{x}), \quad (2.18)$$

where M is the particle mass; $\hat{k}$ is the wave number operator; and d is the period of the periodic potential $V(x)$. By imposing the periodic boundary condition, we obtain the eigenstates $|k\rangle$ for the free particle Hamiltonian H_0 as follows:

$$\psi_k(x) = \langle x|k\rangle = \frac{1}{\sqrt{L}} e^{ikx}, \quad (2.19)$$

$$k = \frac{2\pi}{L} l \quad (l \in \mathbb{Z}), \quad (2.20)$$

where $L = N_{\text{size}}d$ is the system size; and N_{site} is the number of sites.

Below, we consider the matrix representation of the periodic potential $V(x)$ by the eigenstates $|k\rangle$. First, we perform Fourier series expansion of the periodic potential $V(x)$ with the reciprocal lattice vector $K = 2\pi/d$ as follows:

$$V(\hat{x}) = \sum_{m \in \mathbb{Z}} V_m e^{imK\hat{x}}. \quad (2.21)$$

Using Eqs. (2.19) and (2.21), we obtain the matrix element $V_{kk'} = \langle k|V|k'\rangle$ as follows:

$$\begin{aligned} V_{kk'} &= \langle k| \left(\sum_{m \in \mathbb{Z}} V_m e^{imK\hat{x}} \right) |k'\rangle = \langle k| \left(\sum_{m \in \mathbb{Z}} V_m \right) |k' + mK\rangle \\ &= \sum_{m \in \mathbb{Z}} V_m \delta_{k, k' + mK}. \end{aligned} \quad (2.22)$$

Since $V_{kk'}$ takes a nonzero value when $k - k' = mK$ ($m \in \mathbb{Z}$), the matrix V is represented as an block diagonal matrix. Here, from the relation of $(2\pi/L)N_{\text{site}} = K$, we find that there are N_{site} of such blocks. These blocks are labeled with k , which satisfies $k - k' \neq mK$ ($m \in \mathbb{Z}$). This label is called a quasimomentum q , usually taken from the 1st Brillouin Zone (BZ) $[-K/2, K/2)$. For example, when the number of sites is even, i.e., $N_{\text{site}} = 2N'_{\text{site}}$, the quasimomentum q is given as follows:

$$q = \frac{2\pi}{L}l, \quad l = -N'_{\text{site}}, -N'_{\text{site}} + 1, \dots, N'_{\text{site}} - 1. \quad (2.23)$$

By the above, the eigenvalue problem in Eq. (2.17) reduces to the eigenvalue problem for each block matrix $H^{(q)}$, where $H^{(q)}$ is represented as follows:

$$H^{(q)} = \sum_{m, m'} |q + mK\rangle \langle q + mK| (H_0 + V(\hat{x})) |q + m'K\rangle \langle q + m'K|$$

$$= \begin{pmatrix} \ddots & & & & \vdots \\ \cdots & V_{-1} & \frac{\hbar^2(q+K)^2}{2M} + V_0 & V_1 & \cdots \\ & \cdots & V_{-1} & \frac{\hbar^2 q^2}{2M} + V_0 & V_1 & \cdots \\ & & \cdots & V_{-1} & \frac{\hbar^2(q-K)^2}{2M} + V_0 & V_1 & \cdots \\ & & & \vdots & & \ddots \end{pmatrix}. \quad (2.24)$$

2.2.1.1 Bloch state

We put an eigenvalue and an eigenstate of $H^{(q)}$ as $\epsilon_q^{(n)}$, $|q, n\rangle$, respectively, where n is the band index. The eigenstate $|q, n\rangle$ can be represented by the superposition of plane waves $|q + mK\rangle$ as follows:

$$\begin{cases} |q, n\rangle = \sum_{m \in \mathbb{Z}} A_m^{(q, n)} |q + mK\rangle, \end{cases} \quad (2.25)$$

$$\begin{cases} \psi_q^{(n)}(x) = \langle x | q, n \rangle = \frac{1}{\sqrt{L}} \sum_{m \in \mathbb{Z}} A_m^{(q, n)} e^{i(q + mK)x}. \end{cases} \quad (2.26)$$

Here, $|q, n\rangle$ and $\psi_q^{(n)}$ are called the Bloch state and the Bloch function, respectively. Note that if the Schrödinger equation for a considering system is separable for each coordinate, which is true for an optical lattice and an optical superlattice in this work, the above discussion for the 1D potential case can be directly extended to a 3D periodic potential case. In this case, eigenvalues $\epsilon_q^{(n)}$ and eigenstates $\psi_q^{(n)}(\mathbf{x})$ are given as follows:

$$\epsilon_q^{(n)} = \epsilon_{q_x}^{(n_x)} + \epsilon_{q_y}^{(n_y)} + \epsilon_{q_z}^{(n_z)}, \quad \psi_q^{(n)}(\mathbf{x}) = \psi_{q_x}^{(n_x)}(x) \psi_{q_y}^{(n_y)}(y) \psi_{q_z}^{(n_z)}(z). \quad (2.27)$$

We also note that by considering the conversion of the Bloch function in the spatial translation with the period d of the periodic potential $V(x)$, we obtain Bloch's theorem as follows:

$$\psi_q^{(n)}(x+d) = \frac{1}{\sqrt{L}} \sum_{m \in \mathbb{Z}} A_m^{(q,n)} e^{iqd} e^{i(q+mK)x} = e^{iqd} \psi_q^{(n)}(x). \quad (2.28)$$

2.2.1.2 Wannier state

The Bloch state is a superposition of plane waves and is itinerant throughout the system. On the other hand, it is possible to construct a state localized at each site of the periodic potential (potential minima) from the Bloch states. This localized state is called the Wannier state and is defined as the Fourier transform of the Bloch state as follows:

$$|i, n\rangle = \frac{1}{\sqrt{N_{\text{site}}}} \sum_{q \in \text{1st BZ}} e^{-iqx_i} |q, n\rangle, \quad (2.29)$$

where x_i is the coordinate of a site i . Here, $w_i^{(n)}(x) := \langle x|i, n\rangle$ is called the Wannier function. We note that for optical lattices in this work, the Wannier function for a 3D periodic potential is given as a product of Wannier functions for each coordinate as follows:

$$w_{\mathbf{i}}^{(n)}(\mathbf{x}) = w_{i_x}^{(n)}(x) w_{i_y}^{(n)}(y) w_{i_z}^{(n)}(z). \quad (2.30)$$

The Wannier state is defined by Eq. (2.29), but it is not uniquely defined because the Bloch states $|q, n\rangle$ has phase degrees of freedom. In addition, the calculation of on-site interaction strength U in the Hubbard model, which is described below, requires using the Wannier states that are well localized at each site. For a monochromatic optical lattice and an optical superlattice with a relative phase $\phi = \pi/2$, which is used in this work, the phase degrees of freedom of the eigenvectors of $H(q)$ are limited to ± 1 because $H(q)$ is a real symmetric matrix. In this case, to constitute a Wannier state well-localized at each site, the phases for eigenvectors $\mathbf{A}^{(q,n)} = (A_m^{(q,n)})$ of $H(q)$ in Eq. (2.25) should be determined sequentially from $q_{\min} = -K/2$ as the following rule:

$$\mathbf{A}^{(q+\Delta q, n)} = \begin{cases} \mathbf{A}^{(q, n)} & (\|\mathbf{A}^{(q, n)} + \mathbf{A}^{(q+\Delta q, n)}\| > \|\mathbf{A}^{(q, n)} - \mathbf{A}^{(q+\Delta q, n)}\|) \\ -\mathbf{A}^{(q, n)} & (\|\mathbf{A}^{(q, n)} + \mathbf{A}^{(q+\Delta q, n)}\| \leq \|\mathbf{A}^{(q, n)} - \mathbf{A}^{(q+\Delta q, n)}\|), \end{cases} \quad (2.31)$$

where $\|\cdot\|$ denotes the norm of the vector. In this way, the sign of $\mathbf{A}^{(q,n)}$ changes smoothly for q , and the Bloch functions in Eq. (2.29) are added in phase, which leads to a well-localized Wannier state.

2.2.2 Band structure of a monochromatic optical lattice

In the following, we describe an energy band structure of a specific 1D periodic potential. First, we treat a 1D potential for a monochromatic optical lattice. In this case, the optical

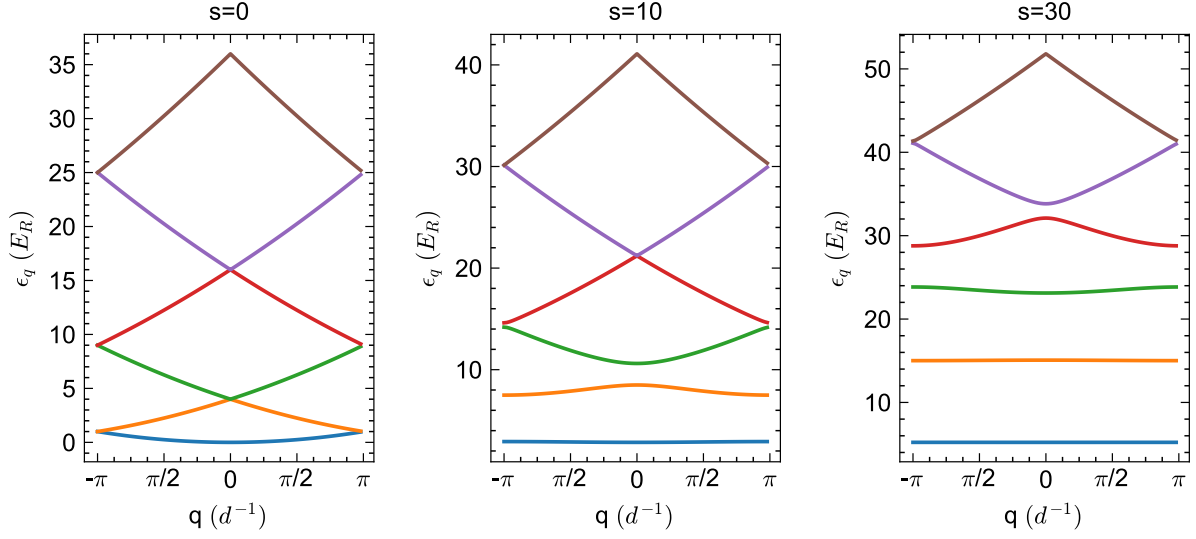


Figure 2.1: Band structures of 1D monochromatic optical lattices. Here, we set $N_{\text{site}} = 101$ and $m_{\text{max}} = 50$ in the calculation.

lattice potential $V(x)$ is given as follows:

$$V(x) = V_0 \sin^2(k_L x) = \frac{V_0}{2} \left(1 - \frac{e^{2ik_L x} + e^{-2ik_L x}}{2} \right), \quad (2.32)$$

where V_0 is the potential depth; and $k_L = 2\pi/\lambda$ is the wave number of the laser creating the optical lattice (wavelength λ). Since the lattice constant of the optical lattice is $d = \lambda/2$ and thus $k_L = K/2$, we obtain the matrix element $H_{mm'}^{(q)}$ of $H^{(q)}$ from Eqs. (2.21), (2.24), and (2.32) as follows:

$$H_{mm'}^{(q)}/E_R = \begin{cases} \left(\frac{q}{k_L} + 2m \right)^2 + \frac{s}{2} & (m = m') \\ -\frac{s}{4} & (m = m' \pm 1) \\ 0 & (\text{otherwise.}), \end{cases} \quad (2.33)$$

where $E_R = \hbar^2 k_L^2 / 2M$ is the recoil energy; and $s = V_0 / E_R$ is the potential depth normalized by the recoil energy. Note that since $H^{(q)}$ is an infinite-dimensional matrix, when we obtain a band structure numerically, we appropriately set the maximum value of m as m_{max} and diagonalize a $(2m_{\text{max}} + 1)$ -dimensional matrix. In Fig. 2.1, we show the band structures of 1D monochromatic optical lattice potentials. Also, in Fig. 2.2, we show the square of the absolute value of the Wannier function constructed by the method described in Sec. 2.2.1.2.

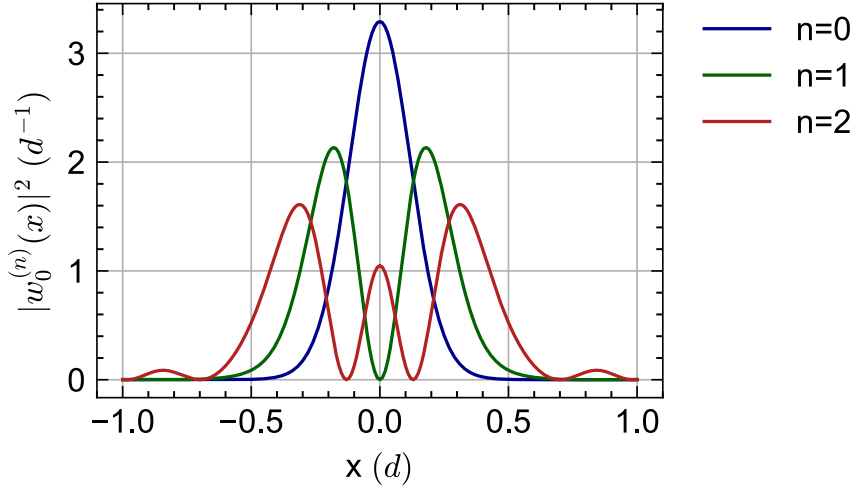


Figure 2.2: Square of the absolute value of the Wannier function $|w_0^{(n)}(x)|^2$ for the lattice depth of $s = 15$. Here, we set $N_{\text{site}} = 101$ and $m_{\text{max}} = 50$ in the calculation.

2.2.3 Band structure of an optical superlattice

Next, we describe an energy band structure of an optical superlattice potential. Here, the optical superlattice is formed by superimposing two optical lattices operating at the wavelength of λ_{long} and $\lambda_{\text{short}} = \lambda_{\text{long}}/2$, and the optical superlattice potential $V(x)$ is given as follows:

$$V(x) = V_{\text{long}} \sin^2(k_L x) + V_{\text{short}} \sin^2(2k_L x + \phi) \quad (2.34)$$

$$= \frac{V_{\text{long}} + V_{\text{short}}}{2} - \frac{V_{\text{long}}}{4} \left(e^{2ik_L x} + e^{-2ik_L x} \right) - \frac{V_{\text{short}}}{4} \left(e^{4ik_L x + 2i\phi} + e^{-4ik_L x - 2i\phi} \right), \quad (2.35)$$

where $V_{\text{short}}(V_{\text{long}})$ is the potential depth of the short (long) lattice created by a laser with the wavelength of $\lambda_{\text{short}}(\lambda_{\text{long}})$; $k_L = 2\pi/\lambda_{\text{long}}$ is the wave number of the long lattice; and ϕ is the relative phase between the short lattice and long lattice. Here, the unit cell of an optical superlattice contains two sites, and the potential shape varies with the relative phase ϕ , as shown in Fig. 2.3. In particular, the condition $\phi = \pi/2$ is called the double-well condition, and the condition $\phi = 0$ is called the staggered condition. In this work, we call an optical superlattice that satisfies the double-well condition a double-well lattice. Since the lattice constant of the optical superlattice lattice is $d = \lambda/2$ and thus $k_L = K/2$, we obtain the

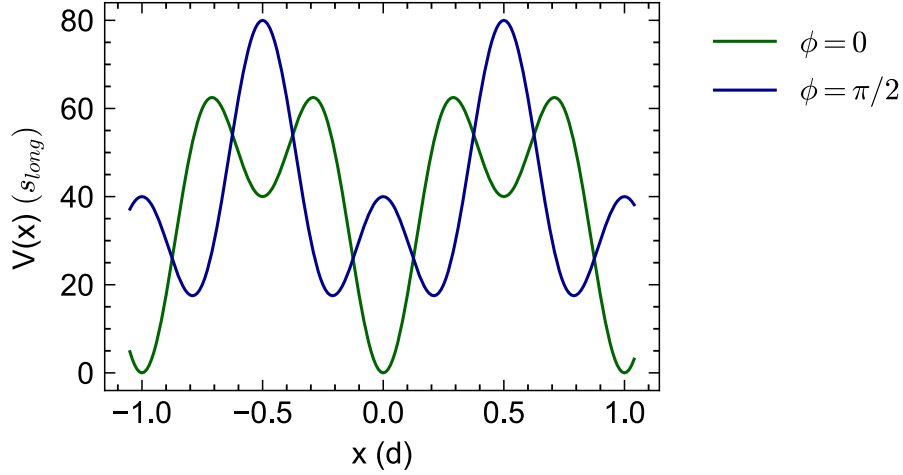


Figure 2.3: Superlattice potential for the double-well condition ($\phi = \pi/2$) and the staggered condition ($\phi = 0$). Here, we set $s_{\text{short}} = s_{\text{long}} = 40E_{\text{R}}^{\text{long}}$ in the calculation.

matrix element $H_{mm'}^{(q)}$ of $H^{(q)}$ from Eqs. (2.21), (2.24), and (2.35) as follows:

$$H_{mm'}^{(q)}/E_{\text{R}}^{\text{long}} = \begin{cases} \left(\frac{q}{k_L} + 2m \right)^2 + \frac{s_{\text{long}} + s_{\text{short}}}{2} & (m = m') \\ -\frac{s_{\text{long}}}{4} & (m = m' \pm 1) \\ -\frac{s_{\text{short}}}{4} e^{2i\phi} & (m = m' + 2) \\ -\frac{s_{\text{short}}}{4} e^{-2i\phi} & (m = m' - 2) \\ 0 & (\text{otherwise.}), \end{cases} \quad (2.36)$$

where $E_{\text{R}}^{\text{long}} = \hbar^2 k_L^2 / 2M$ is the recoil energy for the long lattice; and $s_{\text{short}} = V_{\text{short}} / E_{\text{R}}^{\text{long}}$ and $s_{\text{long}} = V_{\text{long}} / E_{\text{R}}^{\text{long}}$ are the potential depth of the short and long lattice normalized by $E_{\text{R}}^{\text{long}}$, respectively. In Fig. 2.4, we show the band structures of 1D optical superlattice potentials.

2.2.4 Bose-Hubbard & Fermi-Hubbard model

In this section, we briefly introduce the Hubbard model, which describes the ultracold atomic system in an optical lattice. We also describe the expressions of tunneling amplitude t and on-site interaction strength U (Hubbard parameters), which appear in the Hamiltonian of the Hubbard model, for each case of a monochromatic optical lattice (Sec. 2.2.4.2) and an optical superlattice (Sec. 2.2.4.3).

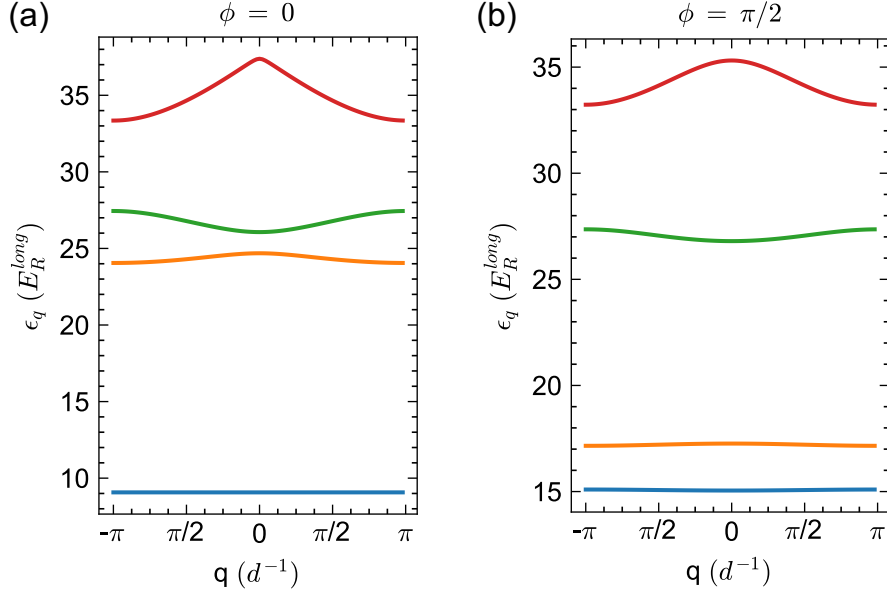


Figure 2.4: Band structures of 1D optical superlattices of $s_{\text{short}} = s_{\text{long}} = 20E_R^{\text{long}}$ in the (a) staggered condition ($\phi = 0$) and (b) in the double-well condition ($\phi = \pi/2$). Here, we set $N_{\text{site}} = 101$ and $m_{\text{max}} = 50$ in the calculation.

2.2.4.1 Hubbard model

The Hubbard model [25, 26], which is a paradigmatic model in condensed matter physics, describes the strongly correlated electron systems, where electrons feel a periodic potential created by atoms in a crystal structure, and interact with each other by Coulomb repulsion. The Hamiltonian for the Hubbard model is given as follows:

$$H = -t \sum_{\langle i,j \rangle, \sigma=\uparrow, \downarrow} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \quad (2.37)$$

where $\hat{c}_{i,\sigma}^\dagger, \hat{c}_{i,\sigma}$ are the fermionic creation and annihilation operators for a site i and spin σ satisfying the anticommutation relation, respectively; $\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}$ is the number operator; t is the tunneling amplitude between nearest-neighbor sites $\langle i, j \rangle$; and U is the on-site interaction strength. Here, the first term on the right-hand side in Eq. (2.37) can be diagonalized using the Bloch functions, which represent an itinerant state throughout the system. On the other hand, the second term can be diagonalized using a number-operator basis, which represents a localized state at each site. Each term in the Hamiltonian of the Hubbard model is simple; however, the competition between the two terms leads to complex behaviors, which, in other words, leads to rich physics. The Hubbard model, though the competition between the itinerancy and localization has made it challenging to fully understand it, has been considered to have a great potential to describe various complex behaviors of quantum many-body systems, especially including the high-temperature

superconductivity [142]. Therefore, more than 60 years after it was proposed, the Hubbard model still lies at the heart of condensed matter physics. Note that the $SU(N)$ Hubbard model, which extends the number of spin components from the usual two to $N(> 2)$ and has enlarged $SU(N)$ symmetry, has also attracted great attention. There, rich quantum phases have been theoretically predicted and also experimentally explored utilizing an intrinsic $SU(N)$ nuclear spin symmetry realized in fermionic isotopes of alkali earth metal-like atoms, such as ytterbium (Yb) and strontium (Sr) [143, 144, 145, 146]

2.2.4.2 Hubbard parameters in a monochromatic optical lattice

The general Hamiltonian describing an ultracold atomic system in an optical lattice in the second quantization representation is given as follows:

$$H = \sum_{\sigma} \int d\mathbf{x} \psi_{\sigma}^{\dagger}(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{lattice}}(\mathbf{x}) + V_{\text{trap}}(\mathbf{x}) \right) \psi_{\sigma}(\mathbf{x}) + \frac{1}{2} \sum_{\sigma, \sigma'} \int d\mathbf{x} d\mathbf{x}' \psi_{\sigma}^{\dagger}(\mathbf{x}) \psi_{\sigma'}^{\dagger}(\mathbf{x}') U(\mathbf{x} - \mathbf{x}') \psi_{\sigma'}(\mathbf{x}') \psi_{\sigma}(\mathbf{x}), \quad (2.38)$$

where $\psi_{\sigma}^{\dagger}(\mathbf{x})$ and $\psi_{\sigma}(\mathbf{x})$ are the creation and annihilation operators of the bosonic or fermionic field at the position $\mathbf{x}$ and spin σ , respectively. Here, $\psi_{\sigma}^{\dagger}(\mathbf{x})$ and $\psi_{\sigma}(\mathbf{x})$ satisfy the commutation relation

$$[\psi_{\sigma}^{\dagger}(\mathbf{x}), \psi_{\sigma'}(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}') \delta_{\sigma, \sigma'}, \quad [\psi_{\sigma}(\mathbf{x}), \psi_{\sigma'}(\mathbf{x}')] = [\psi_{\sigma}^{\dagger}(\mathbf{x}), \psi_{\sigma'}^{\dagger}(\mathbf{x}')] = 0 \quad (2.39)$$

in the case of the bosonic field and the anticommutation relation

$$\{\psi_{\sigma}^{\dagger}(\mathbf{x}), \psi_{\sigma'}(\mathbf{x}')\} = \delta(\mathbf{x} - \mathbf{x}') \delta_{\sigma, \sigma'}, \quad \{\psi_{\sigma}(\mathbf{x}), \psi_{\sigma'}(\mathbf{x}')\} = \{\psi_{\sigma}^{\dagger}(\mathbf{x}), \psi_{\sigma'}^{\dagger}(\mathbf{x}')\} = 0 \quad (2.40)$$

in the case of the fermionic field. On the right-hand side in Eq. (2.38), the first term represents the motion of a single particle in a periodic potential V_{lattice} created by an optical lattice, and a harmonic trap V_{trap} due to lasers for a dipole trap and optical lattices. The second term represents the intrinsic two-body interaction. Here, in an ultracold atomic system, collisions of higher-order partial waves are suppressed by the centrifugal barrier, so the s -wave collisions dominate. In this case, interatomic interaction U is given in the form of the contact interaction and characterized by the s -wave scattering wave a_s as follows:

$$U(\mathbf{x} - \mathbf{x}') = g \delta(\mathbf{x} - \mathbf{x}'), \quad g = \frac{4\pi \hbar^2 a_s}{m}. \quad (2.41)$$

Note that, for the fermionic isotopes of alkali earth metal-like atoms, such as ^{173}Yb and ^{87}Sr , the interaction between the ground-state atoms has enlarged $SU(N > 2)$ symmetry. This is due to no hyperfine interaction in the ground 1S_0 state, i.e., decoupling of the nuclear spin from the electronic spin, which leads to an intrinsic $SU(N = 2I + 1)$ nuclear spin symmetry, where I is the nuclear spin [144, 145].

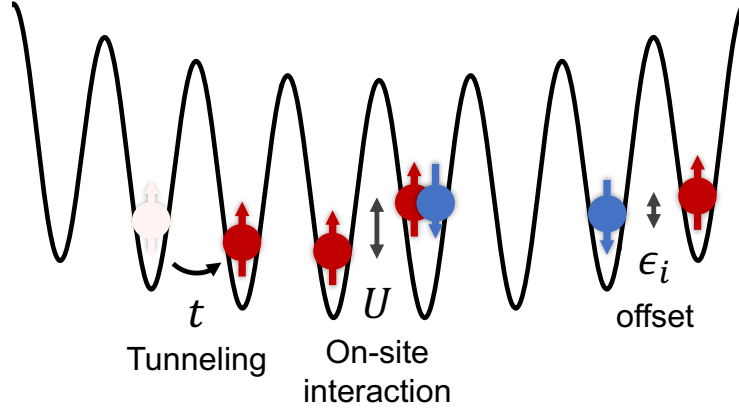


Figure 2.5: Schematic illustration of the Hubbard model.

The expressions of the Hubbard parameters can be obtained by expanding the bosonic or fermionic field operator ψ_σ in Eq. (2.38) by the Wannier functions [27, 28]. Here, we assume that the interatomic interaction and the system temperature are sufficiently smaller than the energy gap between the ground band and the first excited band of the optical lattice potential and that the atoms occupy only the ground band. Under this single-band approximation, we expand the bosonic or fermionic field operator ψ_σ by the Wannier functions of the ground state $\omega_i^{(n=0)}(\mathbf{x})$ as follows:

$$\psi_\sigma(\mathbf{x}) = \sum_i \omega_i^{(0)}(\mathbf{x}) \hat{a}_{i,\sigma}, \quad (2.42)$$

where $\hat{a}_{i,\sigma} = \hat{b}_{i,\sigma} (\hat{c}_{i,\sigma})$ is the bosonic (fermionic) annihilation operator for the bosonic (fermionic) field operator ψ_σ . By substituting Eq. (2.42) into Eq. (2.38), we obtain the following Bose-Hubbard Hamiltonian,

$$H = -t \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i \epsilon_i \hat{n}_i, \quad (2.43)$$

in the case of the bosonic system (with no spin degrees of freedom, as in this work) and the following Fermi-Hubbard Hamiltonian,

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) + \frac{U}{2} \sum_{i, \sigma \neq \sigma'} \hat{n}_{i,\sigma} \hat{n}_{i,\sigma'} + \sum_{i,\sigma} \epsilon_i \hat{n}_{i,\sigma}, \quad (2.44)$$

in the case of the fermionic system (see also Fig. 2.5). Note that in the derivation of Eqs. (2.43) and (2.44), we assume that the atoms are well localized at each site of the periodic potential (tight-binding approximation) and ignore hoppings to sites more distant than nearest-neighbor sites and long-distance interactions other than onsite. These assumptions are known to be valid when the optical lattice potential is relatively deep ($\gtrsim 5E_R$) [28]. The

expressions of the tunneling amplitude t between nearest-neighbor sites, the on-site interaction strength U , and the energy offset ϵ_i in Eqs. (2.43) and (2.44) are given respectively, as follows:

$$t = - \int d\mathbf{x} \omega_i^{(0)*}(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{lattice}}(\mathbf{x}) \right) \omega_{i+1}^{(0)}(\mathbf{x}) \quad (2.45)$$

$$U = \frac{4\pi\hbar^2 a_s}{m} \int d\mathbf{x} \left| \omega_i^{(0)}(\mathbf{x}) \right|^4, \quad (2.46)$$

$$\epsilon_i = \int d\mathbf{x} V_{\text{trap}}(\mathbf{x}) \left| \omega_i^{(0)}(\mathbf{x}) \right|^2 \simeq V_{\text{trap}}(\mathbf{x}_i), \quad (2.47)$$

where $\mathbf{d} = \mathbf{x}_i - \mathbf{x}_{i+1}$; and the approximation in Eq. (2.47) is valid when the harmonic trap potential varies smooth enough. Note that the tunneling amplitude t in Eq. (2.45) can also be written in a form that does not depend on the phase of the Bloch function as follows:

$$\begin{aligned} t &= - \langle i, n=0 | H | i+1, n=0 \rangle \\ &= - \frac{1}{N_{\text{site}}} \sum_{\mathbf{q}} \epsilon_{\mathbf{q}}^{(n=0)} e^{i\mathbf{q} \cdot \mathbf{d}}, \end{aligned} \quad (2.48)$$

where $H = (-\hbar^2/2m)\nabla^2 + V_{\text{lattice}}(\mathbf{x})$. We also note that when the optical lattice potential is sufficiently deep, the following analytical formulae for the Hubbard parameters t and U are known [147]:

$$t/E_R = \frac{4}{\sqrt{\pi}} s^{3/4} e^{-2\sqrt{s}}, \quad U/E_R = \sqrt{\frac{8}{\pi}} k_L a s^{3/4}, \quad (2.49)$$

where k_L is the wave number of the lattice laser; a is the s -wave scattering length; and s is the potential depth of the optical lattice normalized by the recoil energy E_R . More accurate analytical formulae were also obtained in Ref. [148] for the potential depth of an optical lattice of 8-30 E_R as follows:

$$t/E_R = 1.43 s^{0.98} e^{-2.07\sqrt{s}}, \quad U/E_R = 5.97 \frac{a}{\lambda} s^{0.88}, \quad (2.50)$$

where λ is the wavelength of the lattice laser. In Fig. 2.6, we show the dependency of the tunneling amplitude t between nearest-neighbor sites and between next-nearest neighbor sites on the potential depth s of a monochromatic optical lattice.

2.2.4.3 Hubbard parameters in an optical superlattice

The Hamiltonian for the fermionic system in an optical superlattice, which especially satisfies the double-well condition (relative phase $\phi = \pi/2$), is given as follows:

$$H = -t_d \sum_{\langle i,j \rangle_{\text{intra}}, \sigma} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) - t \sum_{\langle i,j \rangle_{\text{inter}}, \sigma} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right) + \frac{U}{2} \sum_{i,\sigma \neq \sigma'} \hat{n}_{i,\sigma} \hat{n}_{i,\sigma'} + \sum_{i,\sigma} \epsilon_i \hat{n}_{i,\sigma}, \quad (2.51)$$

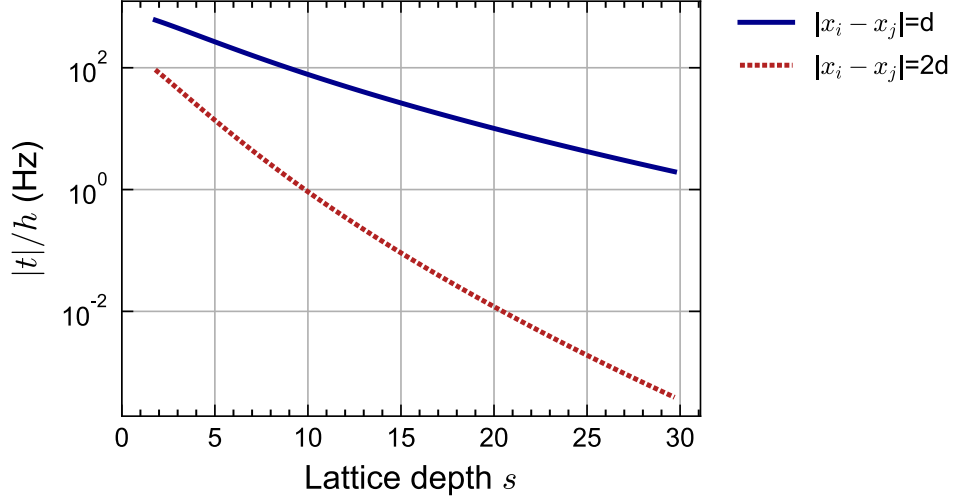


Figure 2.6: Dependency of the tunneling amplitude $|t|/h$ between nearest-neighbor sites (solid curve) and between next-nearest neighbor sites (dotted curve) on the monochromatic lattice depth s .

where t_d and $t(< t_d)$ are the tunneling amplitude between nearest-neighbor sites within double wells $\langle i, j \rangle_{\text{intra}}$ (intra-dimer tunneling) and between double wells $\langle i, j \rangle_{\text{inter}}$ (inter-dimer tunneling), respectively (see Fig. 2.7). Unlike a monochromatic optical lattice, the unit cell contains two sites in the case of an optical superlattice. Therefore, the Wannier states localized at each site in the unit cell cannot be obtained only by the Bloch states in the ground band, and the Bloch states in the first excited band are also needed. Here, to obtain the Wannier states localized at each site in the unit cell, we have to add the Bloch states in the ground band and the first excited band with appropriate coefficients and phases. In this work, we determine these values using an extended tight-binding model, which is described below [149, 150].

In the extended tight-binding model, in addition to the intra-dimer and inter-dimer tunneling, tunnelings between next-nearest-neighbor sites between double wells is also incorporated (see Fig. 2.7). The corresponding Hamiltonian is given as follows:

$$\begin{aligned}
 H_{\text{ETB}} = & -t_d \sum_i \left(\hat{a}_i^\dagger \hat{b}_i + \text{H.c.} \right) - t \sum_i \left(\hat{a}_i^\dagger \hat{b}_{i-1} + \text{H.c.} \right) \\
 & + \sum_{s=a,b} \sum_i \left[-t' \left(\hat{s}_i^\dagger \hat{s}_{i-1} + \text{H.c.} \right) + \epsilon \hat{s}_i^\dagger \hat{s}_i \right],
 \end{aligned} \tag{2.52}$$

where ϵ is the energy offset; t' is the tunneling amplitude between next-nearest-neighbor sites between double wells; and s is the index for the sublattice site. By substituting the following Fourier-transformed creation and annihilation operators into Eq. (2.52),

$$c_i = \frac{1}{\sqrt{N}} \sum_q e^{iqx_{i,S}} c_q, \quad c = a, b, \quad S = A, B, \tag{2.53}$$

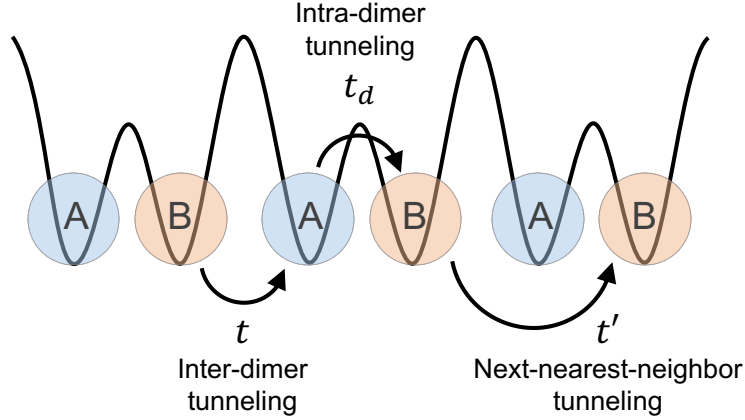


Figure 2.7: Schematic of the extended tight-binding model.

we obtain the diagonalized Hamiltonian with respect to the quasimomentum q as follows:

$$H_{\text{ETB}} = \sum_q \begin{pmatrix} a_q^\dagger & b_q^\dagger \end{pmatrix} T \begin{pmatrix} a_q \\ b_q \end{pmatrix}, \quad (2.54)$$

$$T = \begin{pmatrix} \epsilon - 2t' \cos(qd) & -t_d e^{iqd/2} - t e^{-iqd/2} \\ -t_d e^{-iqd/2} - t e^{iqd/2} & \epsilon - 2t' \cos(qd) \end{pmatrix}, \quad (2.55)$$

where d is the lattice constant of the long lattice. By diagonalizing the matrix T for each quasimomentum q , we obtain the energy dispersion $\epsilon_k^{(n)}$ ($n = 0, 1$) for the parameter sets of t_d , t , t' , and ϵ . In this work, we determine these parameters at each optical superlattice depth so that the band structure of the extended tight-binding model reproduces the band structures of the ground and the first excited band obtained by numerical diagonalization of the Hamiltonian in Eq. (2.36). Here, the three tunneling amplitudes t_d , t and t' , and the energy offset ϵ are determined simultaneously by fitting $\epsilon_k^{(n)}$ ($n = 0, 1$) to the ground and the first excited band of the Hamiltonian in Eq. (2.36).

Using the obtained eigenvectors $u_k^{(n)} = {}^t(u_{k,A}^{(n)} \ u_{k,B}^{(n)})$ of the matrix T , which reflect the appropriate band-mixing between the ground and the first excited band, we obtain the Wannier function well-localized on each sublattice site of an optical superlattice. Here, although there is still a phase degree of freedom in the Bloch functions, these are added in phase at the localized site, by the same method as in the case of the monochromatic optical lattice (see Sec. 2.2.1.2). The Wannier function localized at a site (i, S) is given as follows:

$$w_{i,S}(x) = \sum_q \sum_{n=0}^1 e^{-i\phi(q,n)} e^{-iqx_{i,S}} u_{q,S}^{(n)} \psi_q^{(n)}(x), \quad (2.56)$$

$$\phi(q, n) = \arg \left[e^{-iqx_{i,S}} u_{q,S}^{(n)} \psi_q^{(n)}(x_{i,S}) \right], \quad (2.57)$$

where, the sublattice site $S = A$ or B in the phase $\phi(q, n)$ is chosen to maximize the amplitude $\left| e^{-iqx_{i,S}} u_{q,S}^{(n)} \psi_q^{(n)}(x_{i,S}) \right|$. In Fig. 2.8, we show the square of the absolute value of the

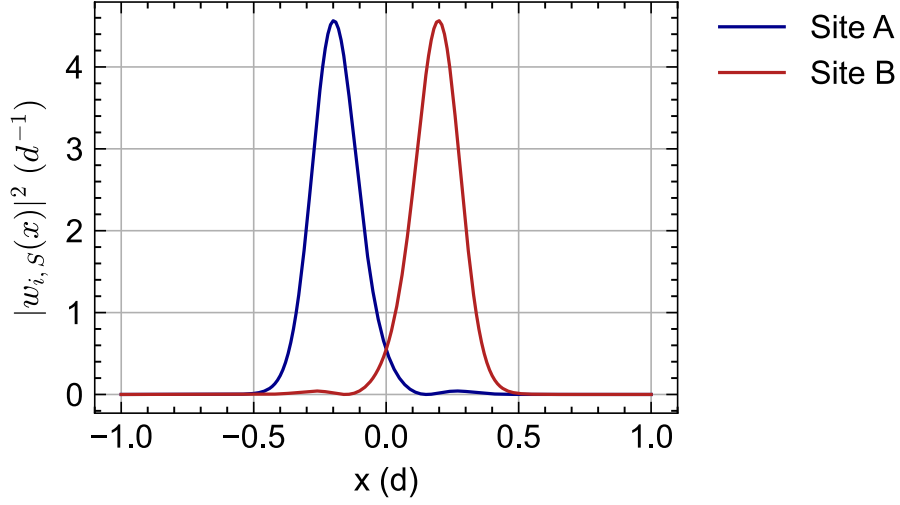


Figure 2.8: Square of the absolute value of the Wannier function well-localized at each sublattice site $|w_{i,S}(x)|^2$ for the lattice depth of $s_{\text{short}} = s_{\text{long}} = 20E_R^{\text{long}}$.

Wannier functions well-localized at each sublattice site constructed by the above method. Using the Wannier function, we also obtain the on-site interaction strength U at each sublattice site as follows, where a double-well lattice exists only along the x direction:

$$U = \frac{4\pi\hbar^2 a_s}{m} \int dx |\omega_{i,S}^{(0)}(x)|^4 \int dy |\omega^{(0)}(y)|^4 \int dz |\omega^{(0)}(z)|^4. \quad (2.58)$$

Note that in the case of $t_d \gg t$, i.e., isolated double-well system, the Wannier function localized at a site (i, S) is given as follows:

$$w_{i,S}(x) = \frac{1}{\sqrt{2}} \left(w_i^{(0)}(x) \pm i w_i^{(1)}(x) \right), \quad (2.59)$$

where $w_i^{(0)}(x)$ and $w_i^{(1)}(x)$ are the Wannier functions constituted by the Bloch functions in the ground band and the first excited band, respectively.

EXPERIMENTAL SETUP

In this chapter, we describe the experimental setup for the optical lattice experiment with trapped ultracold ytterbium (Yb) atoms. First, we describe the general properties of Yb atoms. Then, the trapping and cooling procedure for preparing quantum degenerate gases of Yb is described in Sec. 3.2. In Sec. 3.3, we describe the imaging and the thermometry of trapped gases. In Sec. 3.4, monochromatic optical lattices and optical superlattices are described. In Sec. 3.5, 3.6, we describe the photoassociation (PA) and the optical Stern-Gerlach (OSG) technique, respectively. In Sec. 3.7, and 3.8, we describe a 507 nm laser for the excitation to the metastable 3P_2 state and a 325 nm laser for the ionization from the 3P_2 state, respectively.

3.1 General properties of Ytterbium atoms

Ytterbium (Yb) is an alkali earth metal-like atom with an atomic number of 70. The electronic configuration of ground-state Yb is $[\text{Xe}]4f^{14}6s^2$, where Yb has two valence electrons, as do the alkali earth atoms.

3.1.1 Stable isotopes and s -wave scattering lengths

Yb has seven stable isotopes as listed in Table 3.1, where ^{168}Yb , ^{170}Yb , ^{172}Yb , ^{174}Yb , and ^{176}Yb are bosonic isotopes and ^{171}Yb , ^{173}Yb are fermionic isotopes. The s -wave scattering lengths between each isotope of Yb have been obtained as shown in Table 3.2 [152]. Here, for ^{173}Yb and ^{174}Yb , which are used in this work, s -wave scattering lengths between each isotope is positive, so the interatomic interaction between each atom is repulsive. As mentioned in Sec. 2.2.4.2, the interatomic interaction in the ground state (1S_0) is not dependent on the magnetic sublevels of each atom, so the interaction has enlarged $\text{SU}(N)$ symmetry,

Table 3.1: Basic properties of the seven stable isotopes of Yb [151].

Isotope	Mass (a.u.)	Abundance ratio (%)	Nuclear spin I ($\hbar$)
^{168}Yb	167.933894	0.13	0
^{170}Yb	169.934759	3.05	0
^{171}Yb	170.936323	14.3	1/2
^{172}Yb	171.936378	21.9	0
^{173}Yb	172.938208	16.12	5/2
^{174}Yb	173.938859	31.8	0
^{176}Yb	175.942564	12.7	0

Table 3.2: s -wave scattering lengths between each isotope of Yb (unit: nm) [152].

	^{168}Yb	^{170}Yb	^{171}Yb	^{172}Yb	^{173}Yb	^{174}Yb	^{176}Yb
^{168}Yb	13.33(18)	6.19(8)	4.72(9)	3.44(10)	2.04(13)	0.13(18)	-19.0(1.6)
^{170}Yb		3.38(11)	1.93(13)	-0.11(19)	-4.30(36)	-27.4(2.7)	11.08(12)
^{171}Yb			-0.15(19)	-4.46(36)	-30.6(3.2)	22.7(7)	7.49(8)
^{172}Yb				-31.7(3.4)	22.1(7)	10.61(12)	5.62(8)
^{173}Yb					10.55(11)	7.34(8)	4.22(10)
^{174}Yb						5.55(8)	2.88(12)
^{176}Yb							-1.28(23)

where, in particular, $\text{SU}(2I + 1 = 6)$ symmetry can be realized in the case of ^{173}Yb . So far, a quantum degenerated gas of all bosonic isotopes (a Bose-Einstein condensation) has been generated [153, 154, 155, 156] except for ^{172}Yb , where a BEC is unstable due to its large negative s -wave scattering length. Also, a quantum degenerated gas of both fermionic isotopes (a Fermi degenerate gas) has been generated [157, 158]. Note that enriched stable isotopes of Yb have made possible the various studies using them, such as studies of degenerate mixture gas [159, 155, 158, 160], a new physics search by isotope-shift measurements [161], and a realization of dual-isotope tweezer-array system for quantum computation [162].

3.1.2 Energy levels and transition properties

Energy levels of Yb and their applications in this work are shown in Fig. 3.1. Below, we briefly describe the properties of each transition.

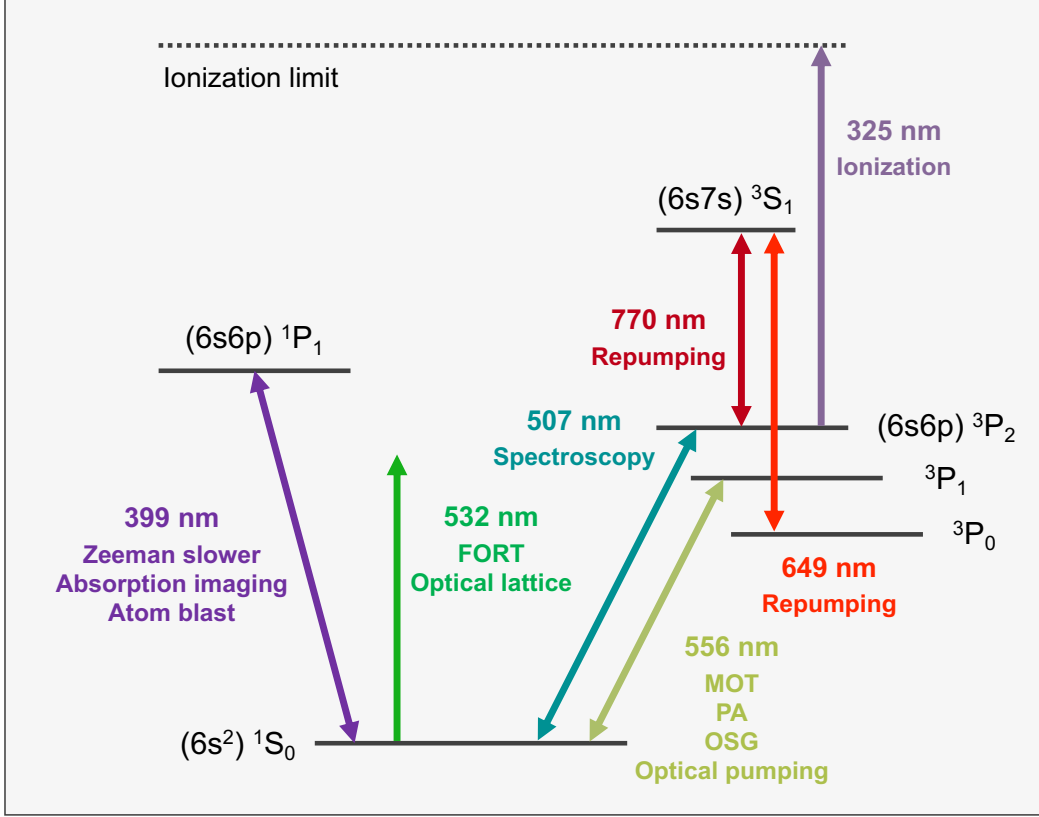


Figure 3.1: Energy levels of Yb and their applications in this work.

- $^1S_0 \leftrightarrow ^1P_1$ transition (399 nm)

This is a strong electric dipole (E1) transition with the natural linewidth of $\Gamma = 2\pi \times 29$ MHz. The basic properties of this transition are shown in Table 3.3. Note that there is a very small but finite branching from the excited 1P_1 state to metastable triplet states (3D_1 and 3D_2 states) with the branching ratio of about 10^{-7} [163]. In this work, this transition is used for a Zeeman slower, absorption imaging, and blasting of the ground-state atoms.

- $^1S_0 \leftrightarrow ^3P_1$ transition (556 nm)

This is an intercombination transition, which is allowed by the mixing with the wave function of the 1P_1 state, with the natural linewidth of $\Gamma = 2\pi \times 182$ kHz. This narrower linewidth leads to a lower Doppler cooling limit of $4.4 \mu\text{K}$, as shown in Table 3.3. In contrast to the $^1S_0 \leftrightarrow ^1P_1$ transition, there is no branching from the 3P_1 state to other states. This property makes the $^1S_0 \leftrightarrow ^3P_1$ transition suitable for the magneto-optical trap since the transition is free from atom losses due to the branching. In this

Table 3.3: Basic properties of the $^1S_0 \leftrightarrow ^1P_1$ and $^1S_0 \leftrightarrow ^3P_1$ transitions [164, 165, 166].

Parameter	$^1S_0 \leftrightarrow ^1P_1$	$^1S_0 \leftrightarrow ^3P_1$	Unit
Wavelength λ	398.9	555.8	nm
Lifetime τ	5.5	873	ns
Linewidth $\frac{\Gamma}{2\pi} = \frac{1}{2\pi\tau}$	29	0.182	MHz
Saturation intensity $I_s = \frac{\pi\hbar c\Gamma}{3\lambda^3}$	59	0.139	mW/cm ²
Doppler cooling limit $T_D = \frac{\hbar\Gamma}{2k_B}$	690	4.37	μ K

work, this transition is used for the magneto-optical trap (MOT) and the photoassociation (PA), and a near-resonant beam is used for the optical Stern-Gerlach (OSG) technique.

- $^1S_0 \leftrightarrow ^3P_2$ transition (507 nm)

This is a magnetic quadrupole (M2) transition whose wavelength is 507.3 nm. A notable feature of this transition is its ultranarrow natural linewidth, which is $\Gamma = 2\pi \times 10.6$ mHz in the bosonic isotope case [167], i.e., the lifetime of the excited 3P_2 state is as long as 15 s. The 3P_2 state has a large magnetic moment of $3\mu_B$ (μ_B : Bohr magneton), which is proposed to be utilized for quantum computing using ultracold Yb atoms in an optical lattice [168, 169]. Also, there exists a magnetic Feshbach resonance in a collision between atoms in the ground 1S_0 state and the metastable 3P_2 ($m_J = +2$) (3P_2 ($m_J = -2$)) state for the bosonic isotope of ^{174}Yb (^{170}Yb) [58]. In this work, this transition is used for the high-resolution spectroscopy in an optical lattice together with the Feshbach resonance, as described in Chapter 4, and also for the removal of atoms in singly occupied sites, as described in Chapter 6.2.5.

- $^3P_2 \leftrightarrow ^3S_1$ & $^3P_0 \leftrightarrow ^3S_1$ transitions (770 nm & 649 nm)

These E1 transitions are used for the detection of atoms in the 3P_2 state. The 770 nm beam and 649 nm beam are used for repumping back atoms from the 3P_2 state and 3P_0 state to the ground state via the 3P_1 state, respectively. Here, the latter beam is

Table 3.4: Basic properties of the $^3P_2 \leftrightarrow ^3S_1$ and $^3P_0 \leftrightarrow ^3S_1$ transitions [167, 80].

Parameter	$^3P_0 \leftrightarrow ^3S_1$	$^3P_1 \leftrightarrow ^3S_1$	$^3P_2 \leftrightarrow ^3S_1$	Unit
Wavelength λ	649.1	680.1	770.2	nm
Radiative decay rate Γ	9.6	27	37	MHz
Branching ratio	0.13	0.37	0.50	

needed due to the branching from the excited 3S_1 state to the metastable 3P_0 state. The basic properties of these transitions are shown in Table 3.4.

3.2 Cooling processes

In this section, we describe the cooling processes of Yb from a thermal atomic gas of 650 ~ 700 K to a quantum degenerate gas of ~ 10 nK, which is performed in an ultra-high vacuum chamber ($\sim 10^{-12}$ Torr).

3.2.1 Zeeman slower

Since Yb is a solid with a low vapor pressure at room temperature, we start by heating and vaporizing it in an atomic oven. As the first step in the cooling process, we cool Yb atoms by a Zeeman slower, where Yb is emitted as an atomic beam from the atomic oven heated to about 650 ~ 700 K. In a Zeeman slower, we irradiate atoms with a counter-propagating resonant laser beam, taking into account the frequency shift caused by the Doppler effect due to the motion of atoms. Here, the atoms are slowed down by absorbing photons and receiving momentum opposite to the motion of the atoms, while the direction of the recoil momentum received from the spontaneously emitted photons is random. As a result, the atoms continue to receive the following average scattering forces as they repeatedly absorb photons [170]:

$$F_{\text{scatt}} = \hbar k \frac{\Gamma}{2} \frac{I/I_{\text{sat}}}{1 + I/I_{\text{sat}} + 4\delta^2/\Gamma^2}, \quad (3.1)$$

where k is the wave number of the laser; Γ is the natural linewidth of the excited state; I/I_{sat} is the laser intensity normalized by the saturation intensity; and $\delta = \omega - \omega_0 - k v$ is the detuning including the Doppler shift $k v$. To compensate for changes in Doppler shift due to the deceleration of the atoms, we apply a magnetic field to induce a position-dependent Zeeman shift to the atoms. Note that in our experimental setup, the magnetic field increases with distance from the atomic oven. This setup has the advantage that the beam for a Zeeman slower is off-resonant at the trapping position of the magneto-optical trap, which is described next, and thus, cooling of the atoms can be performed efficiently.

In this work, we use the $^1S_0 \leftrightarrow ^1P_1$ transition (399 nm. $^1S_0(F = 5/2) \leftrightarrow ^1P_1(F' = 7/2)$ transition for ^{173}Yb case) for a Zeeman slower, which is a strong E1 transition with a short lifetime of 5.5 ns in the excited state. As a laser source of the Zeeman slower, we use a 399 nm beam emitted from a diode laser (Toptica DLC Pro, Toptica Photonics). The laser frequency is locked to an ultra-low-expansion (ULE) cavity by the Pound-Drever-Hall (PDH) scheme. To stabilize the atom number in a prepared atomic sample in each experimental sequence, we also perform the intensity stabilization for the Zeeman slower beam. This is achieved by monitoring the intensity of the Zeeman slower beam with a photodiode and performing a feedback control to the intensity of the input RF signal to an acousto-optic modulator (AOM) installed in the beam path.

3.2.2 Magneto-Optical Trap (MOT)

Yb atoms slowed by a Zeeman slower are subsequently trapped by a Magneto-Optical Trap (MOT). In an MOT, we use three pairs of mutually orthogonal, counter-propagating circularly polarized beams and a quadrupole magnetic field created by two concentric coils (anti-Helmholtz coils) in which opposite currents flow. The magnetic field is zero in the middle of the axis of the two coils (the origin), and the magnetic field gradient varies linearly with the position near the origin. The combination of this magnetic field gradient and counter-propagating circularly polarized beams imposes the following force on atoms near the origin: $F_{\text{MOT}} \simeq -\alpha v - \beta z$ ($\alpha, \beta > 0$, consider only about one direction (z), and valid when Doppler shift and Zeeman shift is much smaller than the natural linewidth Γ). Therefore, it is possible to capture atoms near the zero point of the magnetic field while cooling them.

In this work, we use the $^1S_0 \leftrightarrow ^3P_1$ transition for an MOT (556 nm. $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ transition for ^{173}Yb case), which is an intercombination transition with a narrow linewidth of $\Gamma = 2\pi \times 182$ kHz, and has a Doppler cooling limit of $4.4 \mu\text{K}$. As a laser source of the MOT, we use a 556 nm beam generated through second-harmonic generations (SHG) using a waveguide of periodically poled lithium niobate (PPLN, NTT Electronics), where a fundamental laser at 1112 nm is emitted from a diode laser (Toptica DLC Pro, Toptica Photonics). The frequency and intensity of the MOT laser are stabilized in the same way as the laser for the Zeeman slower. To load atoms into a far-off resonant trap, we ramp up the magnetic-field gradient to increase the atomic density (compressed MOT scheme), then decrease the intensity and detuning of the MOT laser for cooling. Here, we typically obtain about 5×10^6 ^{173}Yb atoms, and about 1×10^7 ^{174}Yb atoms in the MOT after 8 seconds atom loading.

3.2.3 Far-Off Resonant Trap (FORT)

The atoms cooled and trapped by a Zeeman slower and MOT are then further cooled down to the quantum degenerate regime by an all-optical method in a Far-Off Resonant Trap (FORT), which is formed by two lasers in the vertical and horizontal directions in this work.

The FORT is a technique to trap neutral atoms by a far-off resonant laser, utilizing a dipole force acting on the atoms. When a far-off resonant laser is irradiated to an atom, an energy shift called AC Stark shift (or light shift) occurs in the atom as a second-order perturbation. The light shift $U(\mathbf{r})$ induced in the atom is given as follows [171]:

$$U(\mathbf{r}) = -\frac{3\pi c^2 I(\mathbf{r})}{2} \sum_i \frac{1}{\omega_i^3} \left(\frac{\Gamma_i}{\omega_i - \omega} + \frac{\Gamma_i}{\omega_i + \omega} \right) \Big|_{|\delta_i| \ll \omega_i} \simeq \frac{3\pi c^2 I(\mathbf{r})}{2} \sum_i \frac{\Gamma_i}{\omega_i^3 \delta_i}, \quad (3.2)$$

where ω is the angular frequency of the laser; $I(\mathbf{r})$ is the intensity of the laser at position $\mathbf{r}$; and c is the velocity of the light. The summation is taken over all possible transitions i from the state in which the atom is; and ω_i , $\delta_i = \omega - \omega_i$, and Γ_i are the resonant angular frequency, the detuning, and the natural linewidth for each transition i , respectively.

In this work, we use two 532 nm lasers as a FORT in the vertical direction (V-FORT) and the horizontal direction (H-FORT). As laser sources for V-FORT and H-FORT, we use diode lasers (Verdi-V10, Coherent Inc, and Verdi-V18, Coherent Inc, respectively). These beams are Gaussian beams (TEM_{00}), and its intensity profile $I(\mathbf{r})$ is given as follows:

$$I(\mathbf{r}) = \frac{2P}{\pi w^2(z)} \exp\left(-\frac{2\rho^2}{w^2(z)}\right), \quad (3.3)$$

$$w(z) = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2}, \quad (3.4)$$

$$z_R = \frac{\pi w_0^2}{\lambda}, \quad (3.5)$$

where z is the coordinates on the optical axis when the focal point is taken as the origin; ρ is the distance from the optical axis; P is the total power of the beam; w_0 is the beam waist at the focal point; and z_R is the Rayleigh length. Note that a light shift induced in the ground-state (1S_0) Yb atom is given by $U_g(\mathbf{r}) = -\alpha_g I(\mathbf{r})/4$, and the scalar polarizability α_g for a 532 nm beam is calculated to be 37.9 Hz/(Wcm⁻²) [172]. Since the scalar polarizability is positive, Yb atoms are trapped at the focal point where the laser intensity is maximum. Also, a light shift in the magnetic sublevel m_J of the 3P_2 state is given as $U_e(\mathbf{r}) = -\alpha_e(m_J, \theta) I(\mathbf{r})/4$ [173], where

$$\alpha_e(m_J, \theta) = \alpha_e^S - \alpha_e^T (1 - 3\cos^2 \theta) \frac{3m_J^2 - J(J+1)}{2J(J-1)} \quad (3.6)$$

$$= \alpha_e^S - \alpha_e^T (1 - 3\cos^2 \theta) \frac{3m_J^2 - 6}{4}. \quad (3.7)$$

Here, θ is the angle between the quantization axis and the polarization of a laser beam; and α_e^S and α_e^T are the scalar and tensor polarizabilities in the 3P_2 state, respectively. For a 532 nm beam, the ratio of the polarizability $\alpha_e(m_J, \theta)/\alpha_g$ was reported in Ref. [174], as listed in Table 3.5, where the ratio is obtained by spectroscopically determining the band gap in the 3D optical lattice with a 507 nm laser.

Table 3.5: Ratio of the polarizability $\alpha_e(m_J, \theta)/\alpha_g$ [174].

	$\alpha_e(0, \theta)/\alpha_g$	$\alpha_e(-1, \theta)/\alpha_g$	$\alpha_e(-2, \theta)/\alpha_g$
$\theta = 0^\circ$	1.023(10)	-	1.43(5)
$\theta = 90^\circ$	1.32(4)	1.22(8)	1.132(8)

The potential near the center of FORT, i.e., $U(\mathbf{r} \sim \mathbf{0})$, is approximated by a harmonic potential and characterized by trap frequencies as follows:

$$U(\mathbf{r}) \simeq U(\mathbf{0}) \left(1 - \left(\frac{z}{z_R} \right)^2 - 2 \left(\frac{\rho}{w_0} \right)^2 \right) = U(\mathbf{0}) + \frac{1}{2} m (\omega_z^2 z^2 + \omega_\rho^2 \rho^2), \quad (3.8)$$

$$\omega_\rho = \sqrt{\frac{4|U(\mathbf{0})|}{m w_0^2}}, \quad \omega_z = \sqrt{\frac{2|U(\mathbf{0})|}{m z_R^2}}, \quad (3.9)$$

where ω_ρ and ω_z are the radial and axial trap frequencies, respectively, which are typically on the order of $2\pi \times 100$ Hz, and $2\pi \times 10$ Hz, respectively, with the beam waist of several tens of micrometer.

To generate a quantum degenerate gas, we perform an evaporative cooling by gradually decreasing the potential depth of a FORT by reducing the intensity of the FORT beam. Here, the temperature of the atomic gas is decreased by the repetition of loss of atoms with large kinetic energy from the FORT and subsequent thermal equilibration due to elastic collisions between the atoms. In this work, we use a recapture FORT in the horizontal direction (H-ReFORT) in the final evaporative cooling stage to stabilize the atom number of a generated quantum degenerate gas. The laser source of the H-ReFORT is the same as V-FORT (but a frequency offset is added by an acousto-optic modulator), and a fiber-emitted beam is used for the H-ReFORT. Note that the intensity of all FORT beams is stabilized using AOMs. Also, we perform the pointing stabilization of the V-FORT and H-ReFORT beams by monitoring these beam pointings on CCD (Charge Coupled Device) cameras and performing a feedback control to a piezo-transducer (PZT)-mounted mirrors installed in their beam paths. Typically, the evaporative cooling takes about 20 seconds in this work.

3.3 Imaging

In this section, we describe the imaging method of an atomic cloud and the thermometry of trapped atoms.

3.3.1 Absorption imaging

In this work, we perform an absorption imaging, in which we irradiate an atomic cloud with a resonant beam (probe beam), and its shadow is projected on a CCD camera. When

the column density of the atomic cloud integrated along the propagation direction of the probe beam (parallel to the z -axis) is given by $n(x, y) = \int dz n(\mathbf{x})$, the intensity distribution $I(x, y)$ of the transmitted probe beam is given as follows:

$$I(x, y) = I_0(x, y) \exp(-\sigma_{\text{abs}} n(x, y)), \quad (3.10)$$

where $I_0(x, y)$ is the intensity distribution of the probe beam before transmitting the atomic cloud; and σ_{abs} is the absorption cross-section of the atoms. Here, σ_{abs} is given by $3\lambda^2/2\pi$ when a resonant beam of sufficiently weak intensity ($I_0 \ll I_s$, I_s : saturation intensity) is irradiated to a two-level atom [170].

The intensity distribution projected on the CCD surface is given as follows:

$$\tilde{I}(x, y) = \frac{1}{A^2} I_0\left(\frac{x}{A}, \frac{y}{A}\right) \exp\left[-\sigma_{\text{abs}} n\left(\frac{x}{A}, \frac{y}{A}\right)\right], \quad (3.11)$$

where A is a magnification ratio. By also measuring the intensity distribution without an atomic cloud, which is given as $\tilde{I}_0(x, y) = A^{-2} I_0(x/A, y/A)$ and dividing $\tilde{I}$ by $\tilde{I}_0$, we obtain the column density $n(x, y)$ as follows:

$$n\left(\frac{x}{A}, \frac{y}{A}\right) = -\frac{1}{\sigma_{\text{abs}}} \ln\left(\frac{\tilde{I}(x, y)}{\tilde{I}_0(x, y)}\right). \quad (3.12)$$

Note that in an actual image, the position (x, y) is discretized by CCD pixels as (x_i, y_j) , where (i, j) is the index for labeling the CCD pixel. We also note that to eliminate the noise in the obtained intensity distribution, such as a dark current from a CCD pixel and stray light, we also take the following image in addition to an image T_{x_i, y_j} taken with an atomic cloud and a probe beam and a flat image F_{x_i, y_j} taken with a probe beam and no atomic cloud: a dark frame D_{x_i, y_j} taken with neither an atomic cloud nor a probe beam. Using these images, we obtain the column density for each CCD pixel $n(x_i/A, y_j/A)$ as follows:

$$n\left(\frac{x_i}{A}, \frac{y_j}{A}\right) = -\frac{1}{\sigma_{\text{abs}}} \ln\left(\frac{T_{x_i, y_j} - D_{x_i, y_j}}{F_{x_i, y_j} - D_{x_i, y_j}}\right). \quad (3.13)$$

The total atom number N is obtained by adding up the Eq. (3.13) for all CCD pixels as follows:

$$N = \frac{\Delta s}{A^2} \sum_i \sum_j n\left(\frac{x_i}{A}, \frac{y_j}{A}\right), \quad (3.14)$$

where Δs is the pixel size of the CCD.

In this work, we use the $^1S_0 \leftrightarrow ^1P_1$ transition (399 nm. $^1S_0(F = 5/2) \leftrightarrow ^1P_1(F' = 7/2)$ transition for ^{173}Yb case) for an absorption imaging. Note that, in ^{173}Yb case, we set the absorption cross-section to half of that for a two-level atom, taking into account the hyperfine structure in the excited 1P_1 state. As a laser source for the absorption imaging, we use a frequency-doubled beam emitted from an interference-filter stabilized external-cavity diode laser (IFDL) operating at the wavelength of 798 nm (Optoquest), or use a 399 nm beam emitted from a diode laser (Toptica DLC Pro, Toptica Photonics).

3.3.2 Thermometry

To measure the temperature of an atomic cloud, we perform a time-of-flight (TOF) measurement, where we turn off a trapping beam abruptly and perform an absorption imaging after a certain period of free-fall and a ballistic expansion of the atoms. Here, the obtained density distribution of the atomic cloud reflects its initial momentum distribution in the trap. Below, we describe the time evolution of the density distribution of an atomic cloud released from a harmonic trap [175, 176].

First, we denote the initial ($t = 0$) phase-space distribution ($\hbar^3 \times$ phase-space density) of the atomic cloud in the harmonic trap by $f(r, k)$. Here, the phase-space distribution $f(r, k)$, which is given by the following form as seen below:

$$f(\mathbf{r}, \mathbf{k}) = f\left(\frac{\hbar^2 \mathbf{k}^2}{2m} + \sum_i \frac{1}{2} m \omega_i^2 x_i^2\right), \quad (3.15)$$

where $i = x, y$, and z ; and ω_i is the angular frequency of the harmonic trap for the i -axis direction. Since a particle at position $\mathbf{r}_0$ with momentum $\hbar \mathbf{k}_0$ at $t = 0$ moves to position of $\mathbf{r} = \mathbf{r}_0 + \frac{\hbar \mathbf{k}_0}{m} t$ at time t , the density distribution at time t is given as follows:

$$\begin{aligned} n(\mathbf{r}, t) &= \int d\mathbf{r}_0 \int \frac{d\mathbf{k}_0}{(2\pi)^3} f(\mathbf{r}, \mathbf{k}) \delta\left(\mathbf{r} - \left(\mathbf{r}_0 + \frac{\hbar \mathbf{k}_0}{m} t\right)\right) \\ &= \int \frac{d\mathbf{k}_0}{(2\pi)^3} f\left(\mathbf{r} - \frac{\hbar \mathbf{k}_0}{m} t, \mathbf{k}_0\right). \end{aligned} \quad (3.16)$$

Here, from Eq. (3.15), we obtain the following equation:

$$\begin{aligned} f\left(\mathbf{r} - \frac{\hbar \mathbf{k}_0}{m} t, \mathbf{k}_0\right) &= f\left(\sum_i \left\{ \frac{\hbar^2}{2m} (1 + \omega_i^2 t^2) \left[(\mathbf{k}_0)_i - \frac{m \omega_i^2 x_i t}{\hbar (1 + \omega_i^2 t^2)} \right]^2 + \frac{1}{2} m \omega_i^2 \frac{x_i^2}{1 + \omega_i^2 t^2} \right\}\right) \\ &= f(\tilde{\mathbf{r}}, \tilde{\mathbf{k}}_0), \end{aligned} \quad (3.17)$$

where

$$\begin{cases} (\tilde{\mathbf{r}})_i = \frac{x_i}{b_i(t)} \\ (\tilde{\mathbf{k}}_0)_i = b_i(t) \left[(\mathbf{k}_0)_i - \frac{m \omega_i^2 x_i t}{\hbar (1 + \omega_i^2 t^2)} \right] \\ b_i(t) = \sqrt{1 + \omega_i^2 t^2}. \end{cases} \quad (3.18)$$

By substituting Eq. (3.17) into Eq. (3.16), we obtain the following equation:

$$\begin{aligned} n(\mathbf{r}, t) &= \int \frac{d\mathbf{k}_0}{(2\pi)^3} f(\tilde{\mathbf{r}}, \tilde{\mathbf{k}}_0) \\ &= \frac{1}{\prod_i b_i} \int \frac{d\tilde{\mathbf{k}}_0}{(2\pi)^3} f(\tilde{\mathbf{r}}, \tilde{\mathbf{k}}_0) = \frac{1}{\prod_i b_i} n(\tilde{\mathbf{r}}, t = 0). \end{aligned} \quad (3.19)$$

This equation means that the density distribution at time t after releasing from the trap is obtained by scaling the initial density distribution with a factor of $b_i(t) = \sqrt{1 + \omega_i^2 t^2}$. Below, we describe the time evolution of the density distribution of a thermal atomic gas, a Bose-Einstein condensate, and a Fermi degenerate gas.

3.3.2.1 Thermal gas

The phase-space distribution for a thermal atomic cloud is given by the following Maxwell-Boltzmann distribution:

$$f_{\text{MB}}(\mathbf{r}, \mathbf{k}) = N(\beta\hbar\bar{\omega})^3 \exp \left[-\beta \sum_i \left(\frac{\hbar^2 k_i^2}{2m} + \frac{1}{2} m \omega_i^2 x_i^2 \right) \right], \quad (3.20)$$

where N is the total atom number; $\beta = (k_B T)^{-1}$; and $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the trap frequencies. By substituting Eq. (3.20) to Eq. (3.19), we obtain the density distribution after a time-of-flight duration t as follows:

$$n_{\text{MB}}(\mathbf{r}, t) = \frac{N}{(2\pi)^{3/2} \prod_i \sigma_i(t)} \exp \left(-\sum_i \frac{x_i^2}{2\sigma_i^2(t)} \right), \quad (3.21)$$

where $\sigma_i(t) = b_i(t)/\sqrt{m\beta\omega_i^2}$ is the width of the atomic cloud. By integrating $n_{\text{MB}}(\mathbf{r}, t)$ along one axis or two axes, we obtain the following two-dimensional (2D) or one-dimensional (1D) density distributions:

$$n_{\text{MB}}(x, y, t) = \frac{N}{2\pi\sigma_x(t)\sigma_y(t)} \exp \left(-\sum_{i=1}^2 \frac{x_i^2}{2\sigma_i^2(t)} \right), \quad (3.22)$$

$$n_{\text{MB}}(x, t) = \frac{N}{\sqrt{2\pi}\sigma_x(t)} \exp \left(-\frac{x^2}{2\sigma_x^2(t)} \right). \quad (3.23)$$

By fitting to an obtained absorption image with these formulas, we can obtain the total atom number N and the width of the atomic cloud σ_i , and the temperature T is obtained from σ_i and the trap frequency ω_i . Note that the temperature T is obtained only from σ_i as $T = m\sigma_i^2/k_B t^2$ if the TOF time t is long enough ($\omega_i^2 t^2 \gg 1$).

3.3.2.2 Bose Gas

Non-condensed gas

The phase-space distribution for a non-condensed gas (thermal gas. Considering the below T_c case here) is given semi-classically by the following Thomas-Fermi distribution, which is valid when the temperature of the atomic gas T is much larger than the single-particle energy level spacing $\hbar\bar{\omega}$, i.e., $k_B T \gg \hbar\bar{\omega}$:

$$f_{\text{TF}}^{\text{th}}(\mathbf{r}, \mathbf{k}) = \frac{1}{\exp \left[\beta \left(\sum_i \left(\frac{\hbar^2 k_i^2}{2m} + \frac{1}{2} m \omega_i^2 x_i^2 \right) \right) \right] - 1}. \quad (3.24)$$

By substituting Eq. (3.24) to Eq. (3.19), we obtain the density distribution after a time-of-flight duration t as follows:

$$n_{\text{TF}}^{\text{th}}(\mathbf{r}, t) = \frac{1}{\lambda_{\text{dB}}^3 \prod_i b_i(t)} \text{Li}_{3/2} \left[\exp \left(-\sum_i \frac{x_i^2}{2\sigma_i^2(t)} \right) \right], \quad (3.25)$$

where $\lambda_{\text{dB}} = \sqrt{2\pi\hbar^2/mk_B T}$ is the thermal de Broglie wavelength. By integrating $n_{\text{TF}}^{\text{th}}(\mathbf{r}, t)$ along one axis or two axes, we obtain the following 2D or 1D density distributions:

$$n_{\text{TF}}^{\text{th}}(x, y, t) = \frac{N}{2\pi\sigma_x(t)\sigma_y(t)\text{Li}_3(1)} \text{Li}_2 \left[\exp \left(- \sum_{i=1}^2 \frac{x_i^2}{2\sigma_i^2(t)} \right) \right], \quad (3.26)$$

$$n_{\text{TF}}^{\text{th}}(x, t) = \frac{N}{\sqrt{2\pi}\sigma_x(t)\text{Li}_3(1)} \text{Li}_{5/2} \left[\exp \left(- \frac{x^2}{2\sigma_x^2(t)} \right) \right], \quad (3.27)$$

where we have used the following property of the Polylogarithmic function: $\int_{-\infty}^{\infty} dx \text{Li}_{\alpha}(ze^{-x^2}) = \sqrt{\pi} \text{Li}_{\alpha+1/2}(z)$. Note that these density distributions are normalized so that the integration of them in total space gives the total atom number N .

Bose-Einstein Condensate (BEC)

A BEC is described by a many-body wavefunction $\psi(\mathbf{r}, t)$ which obeys the following Gross-Pitaevskii equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + g|\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t), \quad (3.28)$$

where $V(\mathbf{r})$ is the trapping potential; and $g = 4\pi\hbar^2 a/m$, where a is the s -wave scattering length. By substituting the ground-state wave function $\psi(\mathbf{r}, t) = \exp(-i\mu t/\hbar)\psi(\mathbf{r})$ into Eq. (3.28), we obtain the following stationary Gross-Pitaevskii equation:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + g|\psi(\mathbf{r})|^2 \right) \psi(\mathbf{r}) = \mu \psi(\mathbf{r}), \quad (3.29)$$

where μ is identified as the chemical potential. When the total atom number is sufficiently large, and the interaction energy dominates the kinetic energy ($g|\psi(\mathbf{r}, t)|^2 \gg \hbar\omega_{x,y,z}$, Thomas-Fermi limit), we can neglect the kinetic energy term in Eq. (3.29):

$$(V(\mathbf{r}) + g|\psi(\mathbf{r})|^2) \psi(\mathbf{r}) = \mu \psi(\mathbf{r}). \quad (3.30)$$

Under this approximation (Thomas-Fermi approximation), we obtain the density distribution of a BEC as follows:

$$n_{\text{TF}}^{\text{BEC}}(\mathbf{r}) = \max \left[\frac{\mu - V(\mathbf{r})}{g}, 0 \right]. \quad (3.31)$$

For an anisotropic three-dimensional harmonic potential $V(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$, the total atom number $N = \int d\mathbf{r} n_{\text{TF}}^{\text{BEC}}(\mathbf{r})$ becomes

$$N = \frac{8\pi}{15} \left(\frac{2\mu}{m\bar{\omega}^2} \right)^{3/2} \frac{\mu}{g}, \quad (3.32)$$

where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$, and the chemical potential μ becomes as follows:

$$\mu = \frac{1}{2} \hbar \bar{\omega} \left(15Na \sqrt{\frac{m\bar{\omega}}{\hbar}} \right)^{2/5}. \quad (3.33)$$

The density distribution of a BEC after releasing from the trap and ballistically expanding for a duration t is given as follows:

$$n_{\text{TF}}^{\text{BEC}}(\mathbf{r}, t) = \frac{15N}{8\pi \prod_i R_i(t)} \max \left[1 - \left(\frac{x^2}{R_x^2(t)} + \frac{y^2}{R_y^2(t)} + \frac{z^2}{R_z^2(t)} \right), 0 \right], \quad (3.34)$$

where $R_i(t) = b'_i(t) \sqrt{2\mu/m\omega_i^2}$ ($i = x, y, z$); and $R_i = \sqrt{2\mu/m\omega_i^2}$ ($i = x, y, z$) is the Thomas-Fermi radius. Here, the scaling factors $b'_i(t)$ satisfy the following equation:

$$\ddot{b}'_i + \omega_i^2 b'_i - \frac{\omega_i^2}{b'_i b'_x b'_y b'_z} = 0. \quad (3.35)$$

Note that when the trap is axially symmetric with respect to z and cigar-shaped ($\omega_x = \omega_y \equiv \omega_{\perp} \gg \omega_z$), Eq. (3.35) can be solved analytically for $\lambda = \omega_z/\omega_{\perp} \ll 1$, and the scaling factors $b'_{\perp} \equiv b'_x = b'_y$ and b'_z are given as follows [177]:

$$b'_{\perp}(\tau) = \sqrt{1 + \tau^2}, \quad (3.36)$$

$$b'_z(\tau) = 1 + \lambda^2 \left(\tau \arctan \tau - \ln \sqrt{1 + \tau^2} \right), \quad (3.37)$$

where $\tau = \omega_{\perp} t$ is the dimensionless time. By integrating $n_{\text{TF}}^{\text{BEC}}(\mathbf{r}, t)$ along one axis or two axes, we obtain the following 2D or 1D density distributions:

$$n_{\text{TF}}^{\text{BEC}}(x, y, t) = \frac{5N}{2\pi R_x(t) R_y(t)} \left[\max \left[1 - \left(\frac{x^2}{R_x^2(t)} + \frac{y^2}{R_y^2(t)} \right), 0 \right] \right]^{3/2}, \quad (3.38)$$

$$n_{\text{TF}}^{\text{BEC}}(x, t) = \frac{15N}{16R_x(t)} \left[\max \left[1 - \frac{x^2}{R_x^2(t)}, 0 \right] \right]^2. \quad (3.39)$$

For the fitting to an obtained density distribution of an atomic cloud, which consists of condensed atoms and non-condensed atoms, we often use a bimodal function, which is a sum of $n_{\text{TF}}^{\text{BEC}}(\mathbf{r}, t)$ and $n_{\text{TF}}^{\text{th}}(\mathbf{r}, t)$. Here, we can obtain the temperature of the atomic cloud from the fit result of $n_{\text{TF}}^{\text{th}}(\mathbf{r}, t)$. In Fig. 3.2(a), we show a typical absorption image of a ^{174}Yb BEC and the fit result of the bimodal fit to its integrated optical density.

3.3.2.3 Fermi Degenerate Gas

The phase-space distribution for an ideal Fermi gas is given semi-classically by the following Thomas-Fermi distribution:

$$f_{\text{TF}}^{\text{FD}}(\mathbf{r}, \mathbf{k}) = \frac{\mathcal{N}}{\exp \left[\beta \left(\sum_i \left(\frac{\hbar^2 k_i^2}{2m} + \frac{1}{2} m \omega_i^2 x_i^2 \right) - \mu \right) \right] + 1}, \quad (3.40)$$

where μ is the chemical potential; and $\mathcal{N}$ is the spin degrees of freedom. By substituting Eq. (3.40) to Eq. (3.19), we obtain the density distribution at time t as follows:

$$n_{\text{TF}}^{\text{FD}}(\mathbf{r}, t) = -\frac{\mathcal{N}}{\lambda_{\text{dB}}^3 \prod_i b_i(t)} \text{Li}_{3/2} \left[-z \exp \left(-\sum_i \frac{x_i^2}{2\sigma_i^2(t)} \right) \right], \quad (3.41)$$

where $z = e^{\beta\mu}$ is the fugacity. By integrating $n_{\text{TF}}^{\text{FD}}(\mathbf{r}, t)$ along one axis or two axes, we obtain the following 2D or 1D density distributions:

$$n_{\text{TF}}^{\text{FD}}(x, y, t) = \frac{N}{2\pi\sigma_x(t)\sigma_y(t)\text{Li}_3(-z)} \text{Li}_2 \left[-z \exp \left(-\sum_{i=1}^2 \frac{x_i^2}{2\sigma_i^2(t)} \right) \right], \quad (3.42)$$

$$n_{\text{TF}}^{\text{FD}}(x, t) = \frac{N}{\sqrt{2\pi}\sigma_x(t)\text{Li}_3(-z)} \text{Li}_{5/2} \left[-z \exp \left(-\frac{x^2}{2\sigma_x^2(t)} \right) \right], \quad (3.43)$$

where we have used the following property of the Polylogarithmic function: $\int_{-\infty}^{\infty} dx \text{Li}_{\alpha}(ze^{-x^2}) = \sqrt{\pi} \text{Li}_{\alpha+1/2}(z)$. Note that these density distributions are normalized so that the integration of them in total space gives the total atom number N . By fitting to an obtained absorption image with these formulas, we can obtain the total atom number N and the fugacity z . Using the obtained fugacity z , we can obtain the normalized temperature by the Fermi temperature, i.e., T/T_F , as follows:

$$T/T_F = \left(-\frac{1}{6\text{Li}_3(-z)} \right)^{1/3}. \quad (3.44)$$

Also, we can obtain the total entropy S by Eq. (2.15). In Fig. 3.2(b), we show a typical absorption image of a Fermi degenerate gas of six-component ^{173}Yb and the fit results of the Gaussian fit and the Thomas-Fermi fit to the azimuthal average of its optical density.

3.4 Optical lattice system

In this section, we describe the experimental setup for a monochromatic optical lattice and an optical superlattice.

3.4.1 Monochromatic optical lattice

3.4.1.1 Monochromatic optical lattice potential

We can create a periodic potential for atoms by laser beams, an optical lattice, by interfering with counter-propagating laser beams, where a standing wave of light is formed. In an actual experimental setup, we create an optical lattice by interfering with an incident laser beam and the retroreflected one by a mirror. In this work, we create an optical lattice using

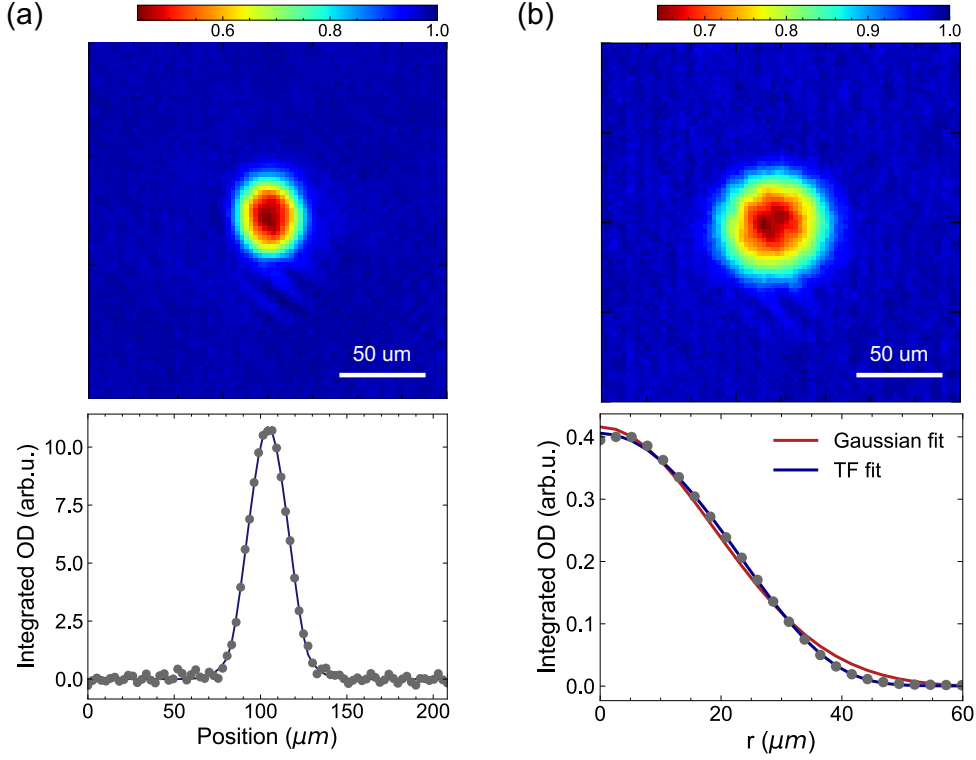


Figure 3.2: Typical absorption images of quantum degenerate gases. (a)(upper) Absorption image of a ^{174}Yb BEC. (a)(lower) Integrated optical density (OD). The solid curve shows the fit result of the bimodal fit, where the total atom number $N = 1.6 \times 10^4$. (b)(upper) Absorption image of a Fermi degenerate gas of six-component ^{173}Yb . (b)(lower) Azimuthal average of OD. The solid curves show the fit results of the Gaussian fit (red) and the Thomas-Fermi fit (Eq. 3.43) (blue), where the total atom number of $N = 2.3 \times 10^4$ and the temperature of $T/T_F = 0.12$ is obtained from the Thomas-Fermi fit.

a Gaussian beam, whose intensity profile is given by Eq. (3.3). In this case, an optical lattice potential $V_{\text{Lattice}}(\mathbf{r})$ (along the z -axis) is given by the following form:

$$V_{\text{Lattice}}(\mathbf{r}) = V_{\text{Lattice}}(\mathbf{0}) \left(\frac{w_0}{w(z)} \right)^2 \exp \left(-\frac{2\rho^2}{w^2(z)} \right) \cos^2(k_L z), \quad (3.45)$$

where k_L is the wave number of the lattice laser. Here, the lattice constant of an optical lattice created by a laser with a wavelength of λ is $\lambda/2$. Note that the term multiplied by $\cos^2(k_L z)$ creates an additional external harmonic confinement in an optical lattice.

In our setup, we can use 532 nm optical lattices along the x -, y -, and z -axes, and 1064 nm optical lattices along the x -, and z -axes, as shown in Fig. 3.3. We also list the beam waists and polarization directions of the 532 nm and 1064 nm optical lattice beams in Table 3.6. Note that the direction of optical lattices along the x - and y -axes is tilted by 45° from the axial direction of the H-FORT and H-ReFORT within the horizontal plane. Here, the intensity of these beams is stabilized using AOMs. As laser sources of the optical lattices, we use a

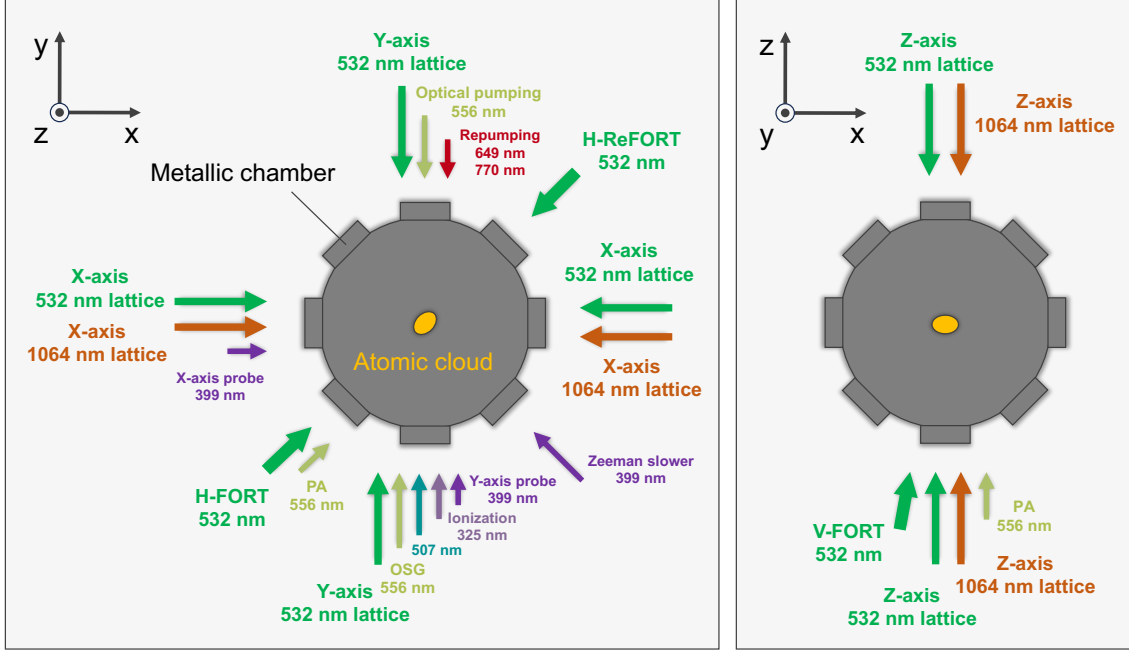


Figure 3.3: Beam paths around the metallic chamber.

532 nm beam emitted from a fiber laser and an amplifier (Azurlight systems) and a 1064 nm beam emitted from a solid-state laser (Mephisto S, Coherent) amplified by a fiber amplifier (Nufern).

In the alignment of the lattice beams, we first align the 532 nm lattice beams, then the 1064 nm lattice beams. In the alignment of the 532 nm lattice beams, we first irradiate a ^{174}Yb BEC trapped in a FORT with a short pulse of the optical lattice beam (typically 2 ms) to give a momentum kick to the atoms, where the retroreflected beam is blocked. If the path is not well-aligned, the atom position after some time-of-flight moves compared to the case without pulse irradiation. Using this, we align the path for the incident lattice beam by measuring the atom position in a TOF image. Then, we align the path of the retroreflected beam with the retroreflection mirror to maximally couple it to a fiber from which the lattice beam is emitted. For the alignment of the 1064 nm lattice beams, we only align the path of the incident beams since the retroreflection mirrors are already aligned in the alignment of the 532 nm lattice beams. Here, we align the path of the incident beam with a mirror to maximally couple it to a fiber from which the lattice beam is emitted.

3.4.1.2 Calibration of the optical lattice potential depth

We calibrate the optical lattice potential depth using a ^{174}Yb BEC by observing the diffraction caused by a pulsed optical lattice [178]. The calibration principle is as follows: we can put the initial state of a condensed atom as $|\psi(t=0)\rangle = |\mathbf{k}=0\rangle$. When we irradiate the atoms

Table 3.6: Parameters for the 532 nm and 1064 nm optical lattices. In 'Polarization', e_i ($i = x, y, z$) is the unit vector parallel to the i -axis.

Wavelength & axis	532- x	532- y	532- z	1064- x	1064- z
Beam waist (μm)	96	120	117	112	128
Polarization	e_z	e_z	e_x	e_z	e_x

with a short pulse of an optical lattice beam, the initial state evolves in time as follows:

$$|\psi(t)\rangle = \sum_n e^{i\omega_n t} |q=0, n\rangle \langle q=0, n|\psi(t=0)\rangle, \quad (3.46)$$

where $|q=0, n\rangle$ is a Bloch state; and $\hbar\omega_n$ is its eigenenergy. Here, if the formed optical lattice potential by the pulse is relatively shallow, it is enough to consider only the two terms corresponding to $n=0, 2$. Note that the term corresponding to $n=1$ has odd parity, which is the opposite parity of the initial state, so this term does not contribute to the dynamics. From these, the state oscillates between the states with the momentum $\mathbf{k}=0$ and $\mathbf{k}=2\mathbf{k}_L$, and we obtain the following time evolution of the probability of the state with the momentum $\mathbf{k}=0$:

$$|\langle\psi(t)|\psi(t=0)\rangle|^2 = 1 - C \sin^2\left(\frac{\omega}{2}t\right), \quad (3.47)$$

where C is a constant value; $\omega = \omega_2 - \omega_0$; and t is the pulse duration.

In the calibration, we observe an oscillation between the 0th- and 1st-order diffraction peaks in a TOF image, which reflects the population of the $0\hbar k$ and $\pm 2\hbar k_L$ momentum components, as a function of the pulse duration. In the case of $15E_R$ lattice depth, the 1st-order diffraction pattern disappears at a pulse duration of about $23.4 \mu\text{s}$ for the 532 nm optical lattice, and about $93.6 \mu\text{s}$ for the 1064 nm optical lattice. In an actual calibration, we fix the pulse duration to these values and change the laser power of the optical lattice, and correspond the laser power at which the 1st-order diffraction pattern disappears to the laser power at $15E_R$.

3.4.2 Optical superlattice

An optical superlattice is formed by superimposing two optical lattices operating at the wavelength of λ_{long} and $\lambda_{\text{short}} = \lambda_{\text{long}}/2$. In this work, we use an optical superlattice formed by a 532 nm beam (short lattice) and a 1064 nm beam (long lattice). Here, the potential of the optical superlattice is given as follows:

$$V(x) = V_{1064} \cos^2(k_{1064}x) + V_{532} \cos^2(2k_{1064}x + \phi), \quad (3.48)$$

where ϕ is the relative phase between the short lattice and the long lattice. Here, to stabilize and control the relative phase ϕ , we measure the beat note between the 532 nm optical lattice beam and the 532 nm beam generated from the 1064 nm optical lattice beam

through SHG using a waveguide of PPLN. Also, we calibrate the relative phase ϕ using a ^{174}Yb BEC by observing the diffraction caused by a pulsed optical lattice, which is similar to the above calibration method of the optical lattice potential depth. Note that these matters, the system for the feedback control of the relative phase and the calibration method of the relative phase, are elaborated on in Ref. [149]. We also note that we can also calibrate the relative phase using a Fermi degenerated gas of ^{173}Yb . In this calibration method, after loading atoms into an optical superlattice, we abruptly turn off the short optical lattice, followed by adiabatic ramping down of the long optical lattice and other optical lattices. Here, the obtained band-mapping image reflects the relative phase: if the relative phase $\phi \neq \pi/2$, there is an imbalance in momentum that the atoms acquire after turning off the short lattice between the atoms at the left and right sites in a double-well lattice, leading to the inhomogeneous density distribution in an obtained image. Using this, we can find a beat frequency that satisfies the double-well condition, where the density distribution becomes homogeneous.

3.5 Photoassociation (PA)

Photoassociation (PA) [179] is a process in which two atoms absorb a single photon when they collide to form an electronically excited molecule with a short lifetime, as depicted in Fig. 3.4. After the PA, the formed short-lived molecule dissociates into two free atoms or transitions to the ground state of the molecule. In the former case, the dissociated two ground-state atoms escape from a trap due to their large kinetic energy. In the latter case, the ground-state molecule is not observed by the absorption imaging with a 399 nm beam. In this work, we utilize the PA technique especially to implement an onsite two-body loss as a dissipation by a laser, as described in Chapter 5, and to measure the quench dynamics in a singlon (atoms in singly occupied sites)- and doublon (atoms in doubly occupied sites)-resolved manner, as described in Chapter 6.

For the PA, we use a 556 nm beam, which is near-resonant to the $^1S_0 \leftrightarrow ^3P_1$ transition ($^1S_0(F=5/2) \leftrightarrow ^3P_1(F'=7/2)$ transition for ^{173}Yb case), generated through SHG using a waveguide PPLN (NTT Electronics), where a fundamental laser at 1112 nm is emitted from a fiber laser (Keopsys). Here, the laser frequency is locked to a ULE cavity by the PDH scheme. We also perform the intensity stabilization for the PA laser using an AOM. The details of the PA transition lines used in each experiment are described in each of the above chapters.

3.6 Optical Stern-Gerlach (OSG) technique

In this section, we describe the Optical Stern-Gerlach (OSG) technique, which is used to observe six nuclear spin components of the ground-state ^{173}Yb ($m_F = -5/2, \dots, +5/2$) in a spatially separated manner using a 556 nm beam (OSG beam). As described in Chapter 5,

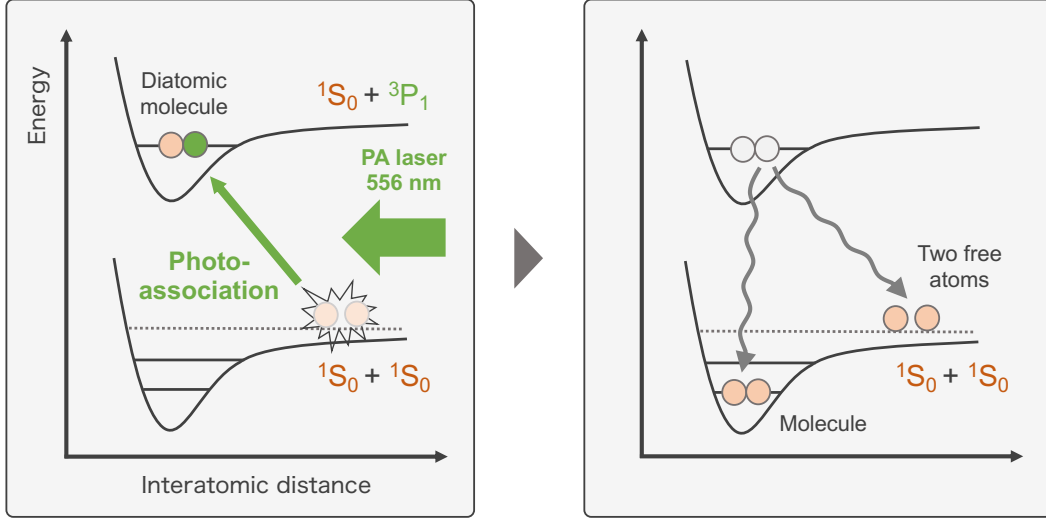


Figure 3.4: Schematic of the PA process.

we also use the OSG beam to induce a singlet-triplet oscillation for a spin pair in an isolated double-well.

For alkali atoms such as sodium, where the spin degree of freedom in the ground-state atom comes from the electron spin, we can spatially separate spin components by the Stern-Gerlach technique, where the magnetic field gradient is applied. On the other hand, for alkali earth metal-like atoms such as Yb, which is used in this work, the spin degree of freedom in the ground-state atom comes from the nuclear spin since the total electronic spin in the ground 1S_0 state is zero. In this case, it is difficult to separate spin components sufficiently in space by the usual Stern-Gerlach technique since the nuclear magnetic moment is about three orders of magnitude smaller than the electron magnetic moment. Therefore, to separate spin components of the alkali-earth-like atoms sufficiently in space, we use the OSG effect [180, 158], where the spin-dependent light shift serves as a fictitious magnetic field.

3.6.1 Dependency of light shifts on magnetic sublevels

The light shift induced in an atom in a ground state of $|F, m_F\rangle$ by irradiating an off-resonant laser is given as follows [181]:

$$\Delta E_{F, m_F} = -\frac{e^2 I}{\epsilon_0 \hbar c} \sum_{F', m_{F'}} \frac{\omega_{F', m_{F'}}}{\omega_{F', m_{F'}}^2 - \omega^2} |\langle F', m_{F'} | r_q | F, m_F \rangle|^2, \quad (3.49)$$

where e is the elementary charge; ϵ_0 is the vacuum permittivity; I and ω are the intensity and the angular frequency of the irradiating laser, respectively; $\omega_{F', m_{F'}}$ is the angular frequency resonant to a transition between a ground $|F, m_F\rangle$ state and an excited $|F', m_{F'}\rangle$

Table 3.7: Resonance frequencies of each $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 3/2, 5/2, 7/2)$ transition for ^{173}Yb with respect to the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ transition [166].

F'	Frequency shift from $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ (GHz)
7/2	0
5/2	4.698
3/2	6.194

state; and $\langle F', m_{F'} | r_q | F, m_F \rangle$ is the dipole matrix element. Here, the dipole matrix element is given as follows by the Wigner-Eckart theorem:

$$\langle F', m_{F'} | r_q | F, m_F \rangle = \langle F' m_{F'} 1 q | F m_F \rangle \frac{\langle \alpha' J' || r || \alpha J \rangle}{\sqrt{2J' + 1}}, \quad (3.50)$$

where $\langle F' m_{F'} 1 q | F m_F \rangle$ is the Clebsch-Gordan coefficient; and $\langle \alpha' J' || r || \alpha J \rangle$ is the reduced dipole matrix element, which is calculated to be $0.54a_0$ (a_0 : Bohr radius) for the $^1S_0 \leftrightarrow ^3P_1$ transition of Yb [167]. In Fig. 3.5, we show the squared values of Clebsch-Gordan coefficients for each $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 3/2, 5/2, 7/2)$ transition, where the resonance frequencies of each transition for ^{173}Yb with respect to the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ transition are listed in Table 3.7. In Fig. 3.6, we show the dependency of the scalar polarizability α_{m_F} for the ground $|F, m_F\rangle$ state of ^{173}Yb on the frequency of the irradiating laser for the cases of linearly polarized light ($q = 0$) and circularly polarized light ($q = +1$), respectively.

Note that, in the case of the linearly polarized light, we obtain a simple integer ratio for the difference of the squared values of the Clebsch-Gordan coefficients, as shown in Table 3.8, since these values only depend on the absolute value of m_F , as shown in Fig. 3.6. Therefore, we obtain the following relation between the difference of the scalar polarizabilities α_{m_F} :

$$\left(\alpha_{\pm\frac{1}{2}} - \alpha_{\pm\frac{3}{2}}\right) : \left(\alpha_{\pm\frac{3}{2}} - \alpha_{\pm\frac{5}{2}}\right) : \left(\alpha_{\pm\frac{1}{2}} - \alpha_{\pm\frac{5}{2}}\right) = 1 : 2 : 3. \quad (3.51)$$

We utilize this relation in the singlet-triplet oscillation method for a six-spin component system, as described in Sec. 5.3.1.

3.6.2 Experimental setup and results

In the OSG technique, we irradiate atoms with a 556 nm pulse at the shoulder of the Gaussian beam after turning off a trap beam to apply a spin-dependent potential gradient at the atom position, which gives the atoms spin-dependent impulses (see Fig. 3.7(a)). Therefore, after a time-of-flight expansion, we can obtain a spatially resolved image of each nuclear spin component. In Fig. 3.7(b), we show a typical spin-resolved image using circularly polarized light with a pulse duration of 0.5 ms, where the frequency of the OSG beam

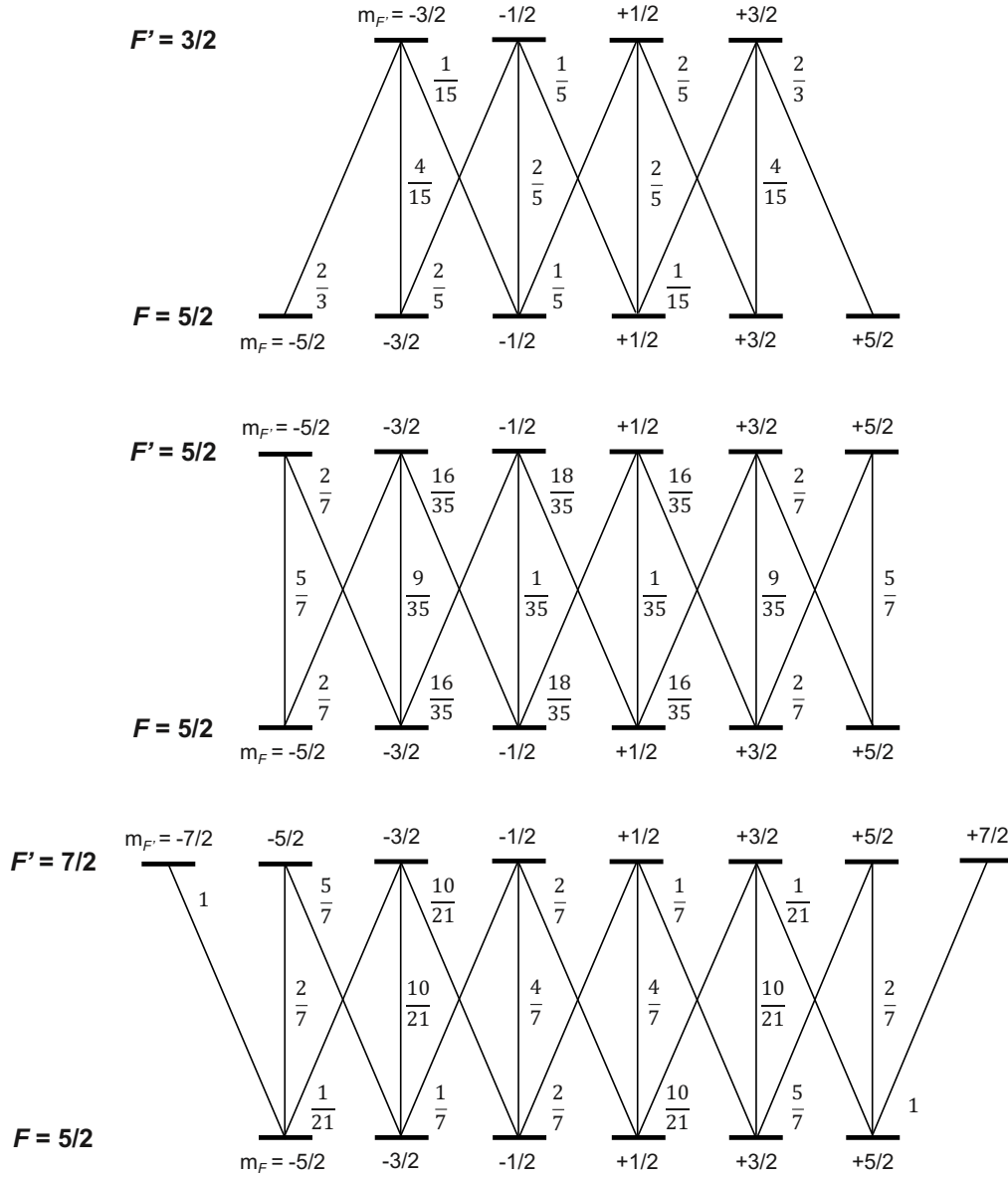


Figure 3.5: Squared values of the Clebsch-Gordan coefficients for the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 3/2)$ transition (upper), the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 5/2)$ transition (middle), and the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ transition (lower).

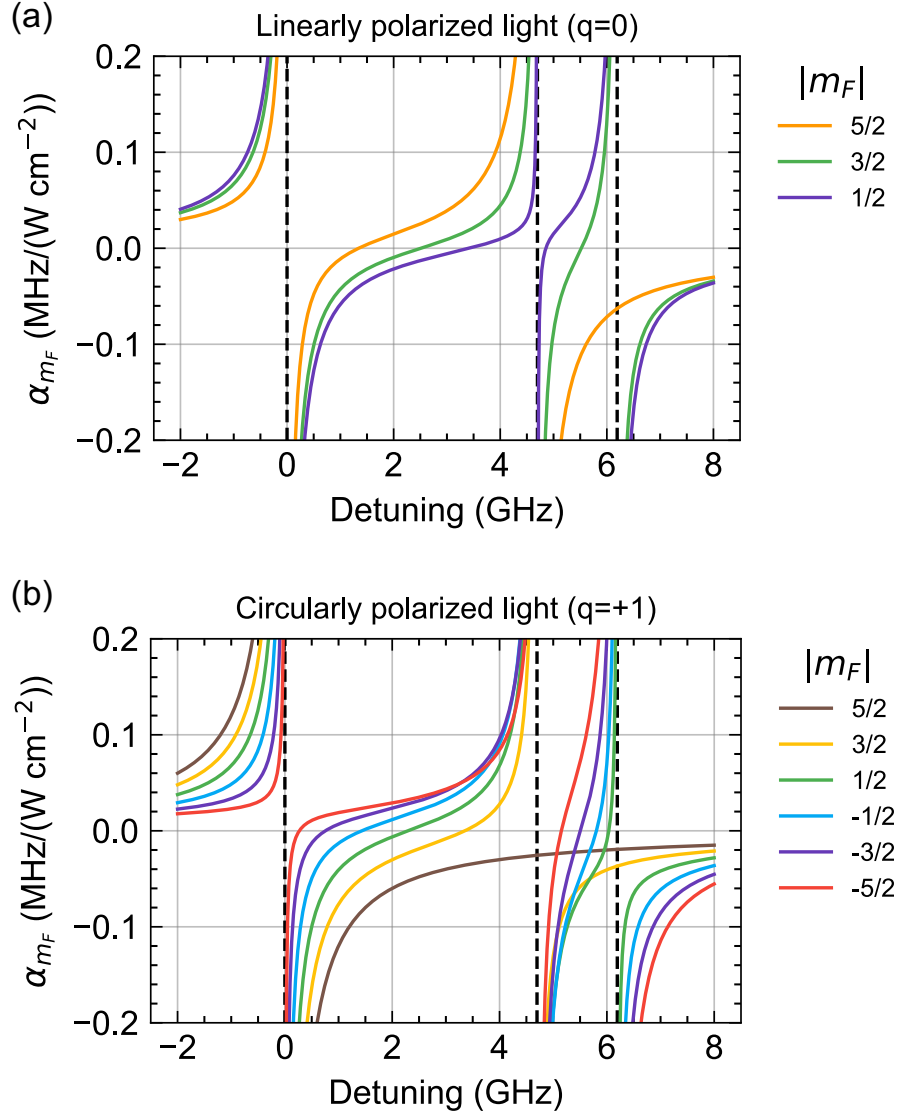


Figure 3.6: Dependency of the scalar polarizability α_{m_F} for the ground $|F, m_F\rangle$ state of ¹⁷³Yb on the frequency of the OSG beam for the cases of (a) linearly polarized light ($q = 0$) and (b) circularly polarized light ($q = +1$). Here, the horizontal axis shows the frequency detuning from the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ transition. The dashed lines show the resonance positions listed in Table 3.7.

Table 3.8: The values of $|\langle F' m_{F',1} 1 q = 0 | F m_F \rangle|^2 - |\langle F' m_{F',2} 1 q = 0 | F m_F \rangle|^2$ for spin pairs of $(|m_{F',1}\rangle, |m_{F',2}\rangle)$ for each $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 3/2, 5/2, 7/2)$ transition. The last line shows the ratio of these values to the one for the spin pair of $(3/2, 1/2)$ for each value of F' .

F'	Spin pairs		
	$(3/2, 1/2)$	$(5/2, 3/2)$	$(5/2, 1/2)$
3/2	-2/15	-4/15	-2/5
5/2	8/35	16/35	24/35
7/2	-2/21	-4/21	-2/7
Ratio	1	2	3

is detuned about +1.4 GHz from the resonant frequency of the $^1S_0(F = 5/2) \leftrightarrow ^3P_1(F' = 7/2)$ transition. Here, a magnetic field of 0.5 G, which defines the quantization axis, is applied along the direction of the propagation of the OSG beam. The OSG beam is generated through SHG using a waveguide PPLN (NTT Electronics), where a fundamental laser at 1112 nm is emitted from a fiber laser (Keopsys). The frequency of the OSG beam is stabilized using a wavemeter (WS7, HighFinesse). We also perform the intensity stabilization for the OSG beam using an AOM.

3.7 507 nm excitation

In this section, we describe the laser system for 507 nm excitation and repumping of the 3P_2 state atoms.

3.7.1 Excitation laser

As the excitation beam, we use a 507 nm beam generated through SHG using a waveguide PPLN (NTT Electronics), where a fundamental laser at 1014 nm is emitted from an IFDL (Optoquest) and amplified by a tapered amplifier (TA) (see Fig. 3.8 for the details of the beam path). Here, the laser frequency is locked to a ULE cavity by the PDH scheme using a commercial laser servo controller (D2-125, Vescent). After passing through an AOM, which is used for the switching and the intensity stabilization, the 507 nm beam is sent to the chamber via a fiber. In this work, we excite atoms by the 507 nm beam from the ground 1S_0 state to the excited 3P_2 ($m_J = 0$) state. Here, we irradiate the atoms with the 507 nm beam, which is linearly polarized parallel to the z -axis, under an applied magnetic field of 0.1 G along the $y - x$ -direction (see Fig. 3.8(b)). The maximum available power of the 507 nm beam just before the chamber window is about 8 mW. The beam waist of the 507 nm beam

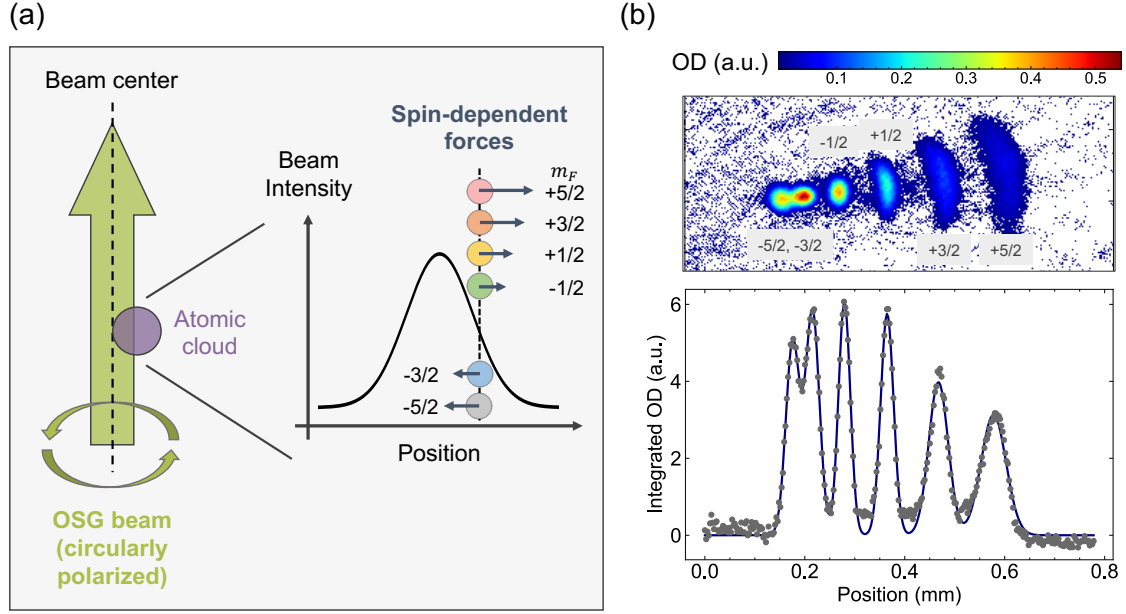


Figure 3.7: OSG technique. (a) Schematic of the OSG technique. (b) Absorption image of six-component ^{173}Yb taken after the OSG beam irradiation (upper) and its integrated OD along the vertical direction (lower). The solid curve in the lower image shows the fit result with a multi-component Gaussian function.

at the atom position is estimated to be $57\ \mu\text{m}$ in the experiment described in Chapter 4, and $31\ \mu\text{m}$ in the experiment described in Chapter 6.

3.7.2 Repumping laser

For the repumping of the 3P_2 state atoms to the ground 1S_0 state, we use a 770 nm beam and a 649 nm beam, which are resonant to the $(6s6p)^3P_2 \leftrightarrow (6s7s)^3S_1$ transition and the $(6s6p)^3P_0 \leftrightarrow (6s7s)^3S_1$ transition, respectively. Both 770 nm beam and 649 nm beam are emitted from IFDLs (Optoquest), where these frequencies are stabilized using a wavemeter (WS8, HighFinesse). After passing through a switching AOM, the 770 nm beam and 649 nm beam are sent to the chamber via a fiber. The powers of the 770 nm beam and 649 nm beam at the fiber output are 3 mW and 2 mW, respectively.

3.8 325 nm laser system

In this section, we describe the laser system for a 325 nm beam, which is used for the one-photon ionization of the 3P_2 state atoms, as described in Sec. 6.2.5. This laser system consists of two parts: a 650 nm laser and an SHG cavity. For a 650 nm seed laser, we use a homemade external cavity diode laser (ECDL), where its frequency is stabilized using a

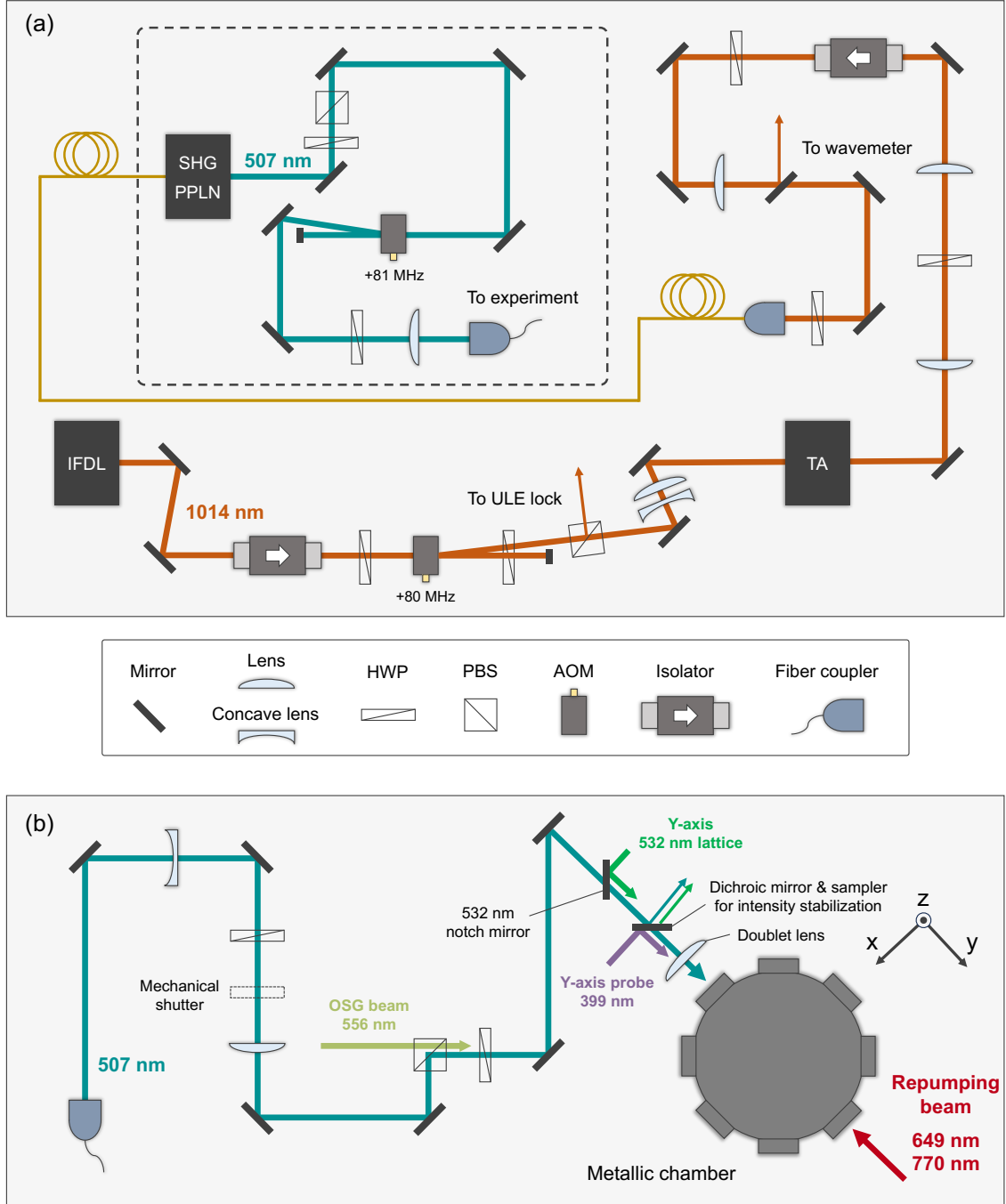


Figure 3.8: Beam paths for the 507 nm beam around (a) the IFDL and the SHG PPLN, and (b) the metallic chamber.

wavemeter (WS8, HighFinesse). The light from the ECDL is amplified by a TA, where the amplified power is about 120 mW when the input power is 20 mW.

The amplified light enters the cavity after passing through an isolator and lens and then is doubled in frequency by SHG (see Fig. 3.9 for the details of beam paths). Here, the SHG cavity is a homemade bow-tie cavity in which a Beta-barium borate (BBO) crystal (Raicol Crystals) is mounted. The measured cavity Finesse (free spectral range divided by the full width at half maximum of the resonance spectrum) is 384, which is roughly close to the estimated value of 447. We perform the cavity lock, namely, stabilization of the cavity length with a PZT-mounted mirror so that the input laser is resonant to the cavity, by the Hänsch-Couillaud method [182]. Here, the power of the emitted 325 nm beam is 1.3 mW under the cavity lock. The generated 325 nm beam is sent to the chamber after beam shaping and passing through a switching AOM, as shown in Fig. 3.9. The power of the 325 nm beam just before the chamber window is about 0.8 mW, and the estimated beam waist at the atom position is 50 μm .

We observe the loss of the 3P_2 state atoms when irradiated with the 325 nm beam in a 3D optical lattice, as shown in Fig. 3.10 (b,c). In this measurement, we first prepare a Mott insulating state of unit filling in a 3D cubic optical lattice operating at 532 nm with a lattice depth of 30 E_R . Then, we irradiate atoms with a π -pulse of a 507 nm beam in 0.16 ms to excite the atoms to the 3P_2 ($m_J = 0$) state, followed by the irradiation of a 325 nm beam, which is linearly polarized parallel to the z -axis, with variable duration to ionize the 3P_2 state atoms. Here, we set the frequency of the 325 nm beam to around the frequency corresponding to the energy difference between the ionization limit and the 3P_2 state. Finally, we irradiate the atoms with a 399 nm beam (blasting beam) in 0.1 ms to remove the remaining ground-state atoms, followed by the irradiation of repumping beams (770 nm and 649 nm beam) in 1.2 ms. We then measure the atom number by absorption imaging (see Fig. 3.10(a) for the timing diagram of this measurement). As shown in Fig. 3.10 (b,c), we observe the loss of the 3P_2 state atoms at a rate of about 3 kHz for the 325 nm beam intensity of 23 W/cm², which is achieved by the above beam power and beam waist. Note that the loss of the 3P_2 state atoms without 325 nm beam irradiation is negligibly small within the uncertainty. We also note that the loss of the ground state atoms when irradiated with the 325 nm beam is negligibly small within the uncertainty, which is a necessary condition to remove only atoms in singly occupied sites by a method described in Sec. 6.2.5.

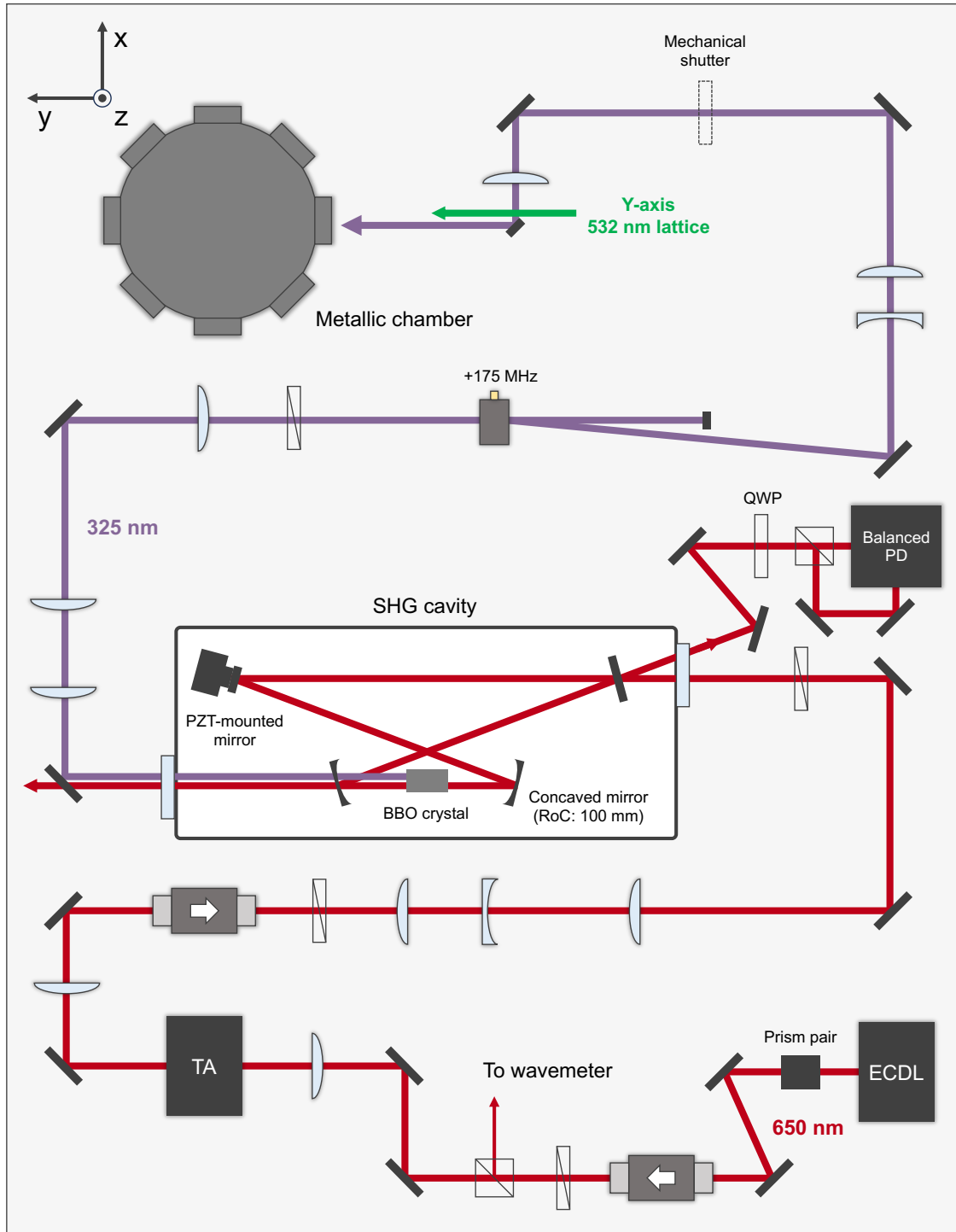


Figure 3.9: Beam paths for the 325 nm beam around the SHG cavity and the metallic chamber.

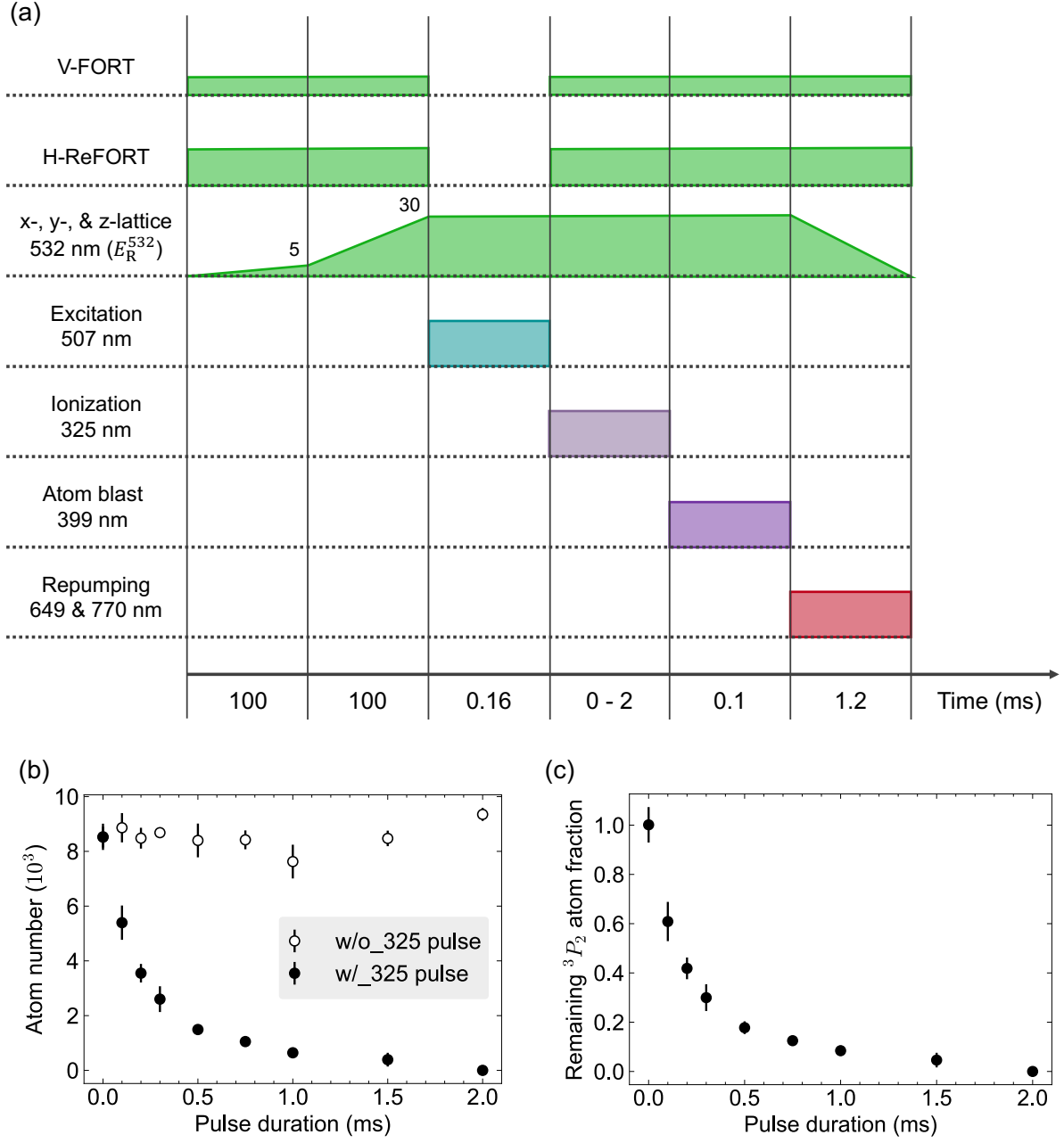


Figure 3.10: Loss of the 3P_2 state atoms by irradiating with a 325 nm beam. (a) Timing diagram of this measurement. (b) Time evolution of the remaining 3P_2 state atoms with the 325 nm pulse irradiation (solid circle) and without pulse irradiation (open circle). (c) The fraction of the atom number with pulse irradiation to that with no pulse irradiation, which is calculated from the results in (b). Error bars represent the standard deviation of three independent scans. Note that we set the atom number at the pulse duration of 2.0 ms to zero since no atom was observed within the uncertainty.

EXPLORING THE STRONGLY-INTERACTING REGIME OF EFFECTIVE MULTI-BODY INTERACTIONS IN A TRAPPED ULTRACOLD ATOM SYSTEM

In this chapter, we report an experimental study of the effective multi-body interaction in a trapped ultracold atom system. By combining occupancy-resolving high-resolution laser spectroscopy with an inter-orbital Feshbach resonance controlling the bare two-body interaction over a wide range, we experimentally reveal the behaviors of few-atom systems in a strongly-interacting regime. In Sec. 4.1, we first describe two theoretical descriptions of ultracold bosons tightly confined in a harmonic trap: microscopic description and effective description. Then, in Sec. 4.2, we describe the sample preparation and show a typical spectroscopic result. In Sec. 4.3, we show the experimental results: variation of resonance-frequency shifts via a Feshbach resonance and effective multi-body interactions in a strongly-interacting regime. Theoretical calculations were performed by Dr. Yusuke Nishida.

4.1 Harmonically trapped bosons

First, we present theoretical descriptions of ultracold bosons tightly confined in a harmonic trap. There are microscopic and effective descriptions, both of which should give the same results. Note that the hopping between neighboring sites is negligible for a sufficiently deep optical lattice potential, and the trapping potential for atoms in each lattice site is well approximated by a harmonic potential.

4.1.1 Microscopic description

The system consisting of multiple bosons in the ground g and excited e states is described by the second-quantized Hamiltonian, on the one hand,

$$\hat{H} = \int d\mathbf{r} \left[\sum_{\sigma=g,e} \hat{\phi}_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{m}{2} \omega^2 \mathbf{r}^2 \right) \hat{\phi}_{\sigma}(\mathbf{r}) + \sum_{\sigma,\sigma'} \frac{g_{\sigma\sigma'}}{2} \hat{\phi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\phi}_{\sigma'}^{\dagger}(\mathbf{r}) \hat{\phi}_{\sigma'}(\mathbf{r}) \hat{\phi}_{\sigma}(\mathbf{r}) \right], \quad (4.1)$$

where m is the mass of the boson; $g_{\sigma\sigma'} = 4\pi\hbar^2 a_{\sigma\sigma'} / m + O(a^2)$ is the coupling constant characterizing the bare two-body interaction via a scattering length $a_{\sigma\sigma'}$; ω is the trap angular frequency which is now assumed to be isotropic and equal before and after the excitation; and $\hat{\phi}_{\sigma}^{\dagger}(\mathbf{r})$ and $\hat{\phi}_{\sigma}(\mathbf{r})$ are the creation and annihilation operators of bosons for the state $\sigma = g, e$, respectively. While only the two-body interaction term exists in Eq. (4.1), we can evaluate, in principle, any physical quantities, including the binding energies of multiple bosons with this Hamiltonian.

4.1.2 Effective description

On the other hand, we also have another useful low-energy effective description by regarding the system as zero-dimensional bosons where we do not consider their spatial degrees of freedom. This description is justified for the case where the energy scale determined by the trap frequency is largest among others like the atom temperature and chemical potential. The effective zero-dimensional Hamiltonian up to five atoms, including up to one excited-state atom, reads

$$\begin{aligned} \hat{H}_{\text{eff}} = & U_g \hat{b}_g^{\dagger} \hat{b}_g + U_e \hat{b}_e^{\dagger} \hat{b}_e + \frac{U_{gg}}{2!} \hat{b}_g^{\dagger 2} \hat{b}_g^2 + U_{eg} \hat{b}_e^{\dagger} \hat{b}_e \hat{b}_g^{\dagger} \hat{b}_g \\ & + \frac{U_{ggg}}{3!} \hat{b}_g^{\dagger 3} \hat{b}_g^3 + \frac{U_{egg}}{2!} \hat{b}_e^{\dagger} \hat{b}_e \hat{b}_g^{\dagger 2} \hat{b}_g^2 + \frac{U_{gggg}}{4!} \hat{b}_g^{\dagger 4} \hat{b}_g^4 \\ & + \frac{U_{eggg}}{3!} \hat{b}_e^{\dagger} \hat{b}_e \hat{b}_g^{\dagger 3} \hat{b}_g^3 + \frac{U_{ggggg}}{5!} \hat{b}_g^{\dagger 5} \hat{b}_g^5 + \frac{U_{egggg}}{4!} \hat{b}_e^{\dagger} \hat{b}_e \hat{b}_g^{\dagger 4} \hat{b}_g^4, \end{aligned} \quad (4.2)$$

where $\hat{b}_{\sigma}^{\dagger}$ and $\hat{b}_{\sigma}$ are the creation and annihilation operators of bosons in the vibrational ground state of a harmonic trap, respectively. Effective multi-body interaction energies entering the effective zero-dimensional Hamiltonian in Eq. (4.2) can be determined by matching the energies of N atoms with those computed from Eq. (4.1).

Note that Effective multi-body interactions have also been of considerable interest in different contexts of the study of localized spin models. Effective multi-spin interactions, arising from higher-order processes of pairwise exchange interactions, were theoretically proposed to explain the magnetic behaviors in solid helium [183] and some organic compounds [184]. In addition, similar effective multi-spin interactions have been recently engineered in artificial systems of a chain of ions in an ion trap [185] and localized spins loaded

into an optical lattice with unit filling [186], which would play an important role in quantum computation and quantum information. Moreover, an effective three-body interaction for photons is successfully implemented by exploiting Rydberg interactions [187].

We also note that, in addition to the effective multi-body interactions, *fundamental* multi-body interactions emerge due to the self-interaction of gluons in the microscopic description of quantum chromodynamics (QCD), and multi-pion interactions naturally lead to the fundamental multi-body interactions also for nucleons [188]. Since such self-interaction is absent for photons, multi-body interactions in atomic and molecular systems only emerge in the low-energy effective description by tracing out the high-energy degrees of freedom involved in the microscopic description.

4.2 Experimental setup

4.2.1 Occupancy-resolving spectroscopy.

4.2.1.1 Sample preparation

Our experiment starts with the preparation of ^{174}Yb Bose-Einstein condensate (BEC) by evaporative cooling in a crossed dipole trap operating at a wavelength of 532 nm. Here, the atom number of BEC is about 3×10^4 . Then, we load it finally into a 3D cubic optical lattice at the potential depth for each axis of the 3D optical lattice of $25 E_R$, where $E_R = \hbar^2 k_L^2 / (2m)$ is the recoil energy of the optical lattice, $k_L = 2\pi / \lambda$ with $\lambda = 532$ nm is the wave number of the laser for the optical lattice, and $\hbar$ is the Planck constant divided by 2π . At this condition, the hopping between neighboring sites is negligible compared with the typical measurement time of 1 ms, and thus, this system can be regarded as an ensemble of various isolated quantum few-body systems with a fixed number of particles at each site.

In this study, in order to prepare sites with a large number of occupied atoms up to five, a staggered-phase optical superlattice is used in the initial loading to the optical lattice, as follows (see Fig. 4.1):

(1) Atoms are loaded adiabatically into the optical lattice at a potential depth of $s_L = [(s_{\text{short}}^{(x)}, s_{\text{long}}^{(x)}), s_{\text{short}}^{(y)}, (s_{\text{short}}^{(z)}, s_{\text{long}}^{(z)})] = [(0, 10), 25, (0, 10)]$ in 300 ms, where $s_{\text{short}}^{(x,y,z)}$ and $s_{\text{long}}^{(x,z)}$ are the potential depth of the short lattice (wavelength $\lambda_{\text{short}} = 532$ nm) and the long lattice ($\lambda_{\text{long}} = 1064$ nm) normalized by the recoil energy for each wavelength, respectively. Here, the atoms are delocalized over lattice sites.

(2) We ramp up the short lattice to $s_L = [(5, 20), 25, (5, 20)]$ in 10 ms and trap atoms in an optical superlattice in a staggered phase (the relative phase between the short and long lattices is zero), where the potential difference between the two sites in the unit cell of the superlattice is maximized, for the x and z directions. Here, the atoms are localized at each lattice site. Note that the potential difference between adjacent sites in a unit cell of an optical superlattice helps to create sites with large occupancy.

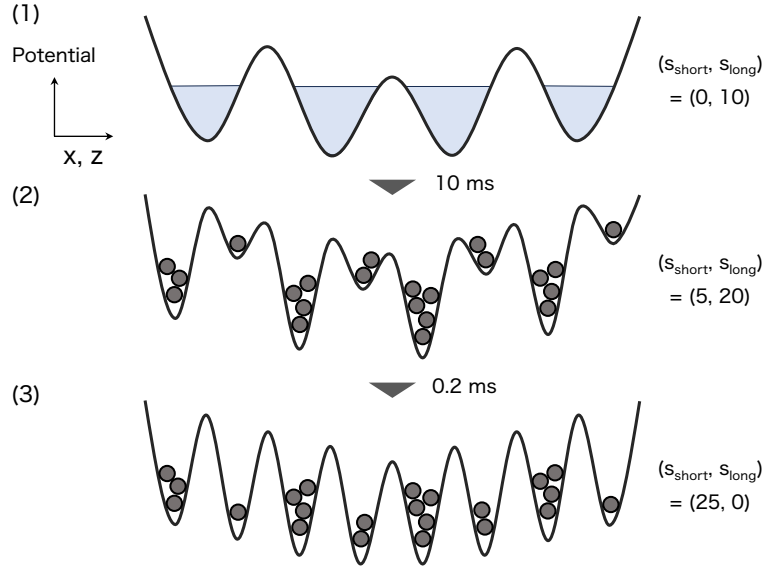


Figure 4.1: Schematic illustration of atom loading schemes using optical superlattice. s_{short} and s_{long} are the potential depth of the short lattice (wavelength $\lambda_{\text{short}} = 532$ nm) and the long lattice ($\lambda_{\text{long}} = 1064$ nm) normalized by the recoil energy for each wavelength, respectively. (1) First we load a ^{174}Yb BEC to a relatively shallow long lattice along the x - and z -axes as well as the tight short lattice along the y -axis. (2) Next, we ramp up a short lattice in 10 ms and trap the atoms in an optical superlattice in a staggered phase, where the atoms are localized at each lattice site. (3) Finally, we quickly ramp up the short lattice in 0.2 ms, while we ramp down the long lattice at the same time, where we use the atom-number-projection technique [189] to increase the number of sites with large atomic occupancy.

(3) The short lattice is quickly ramped up to the final potential depth of $s_L = [(25, 0), 25, (25, 0)]$ in 0.2 ms, while at the same time the long lattice is ramped down. Here, we use the atom-number-projection technique [189], which is also helpful to increase the number of sites with large atomic occupancy.

After loading atoms into the optical lattice, the dipole trap is turned off to reduce spatial inhomogeneity of the trapping potential, and the atoms are trapped only by the optical lattice potential, followed by the irradiation of the excitation laser.

In the configuration of our optical lattice system, the trap angular frequencies for atoms in the ground 1S_0 and excited 3P_2 ($m_J = +2$) states are $\omega_g = 2\pi \times (35.9, 35.9, 35.9)$ kHz and $\omega_e = 2\pi \times (44.0, 44.0, 38.5)$ kHz, respectively, at the final potential depth of $25 E_R$. Here, these trap angular frequencies are determined as the average band gaps from the optical lattices with $\lambda = 532$ nm, $\mathbf{s}_g = 25 \times (1, 1, 1)$, and $\mathbf{s}_e = 25 \times (1.43, 1.43, 1.132)$.

4.2.1.2 Typical spectroscopic results

After loading BEC into an optical lattice, high-resolution laser spectroscopy of the ultra-narrow magnetic quadrupole $^1S_0 \leftrightarrow ^3P_2$ transition is performed. First, a laser pulse resonant to the $^1S_0 \leftrightarrow ^3P_2$ ($m_J = +2$) transition, whose wavelength is 507 nm, is irradiated for 1.0 ms. The optical lattice is then adiabatically lowered to transfer atoms into an optical dipole trap, and absorption imaging is performed to measure the number of atoms remaining in the ground 1S_0 state. A typical spectrum obtained in this manner is shown in Fig. 4.2 (upper), where the signals corresponding to different numbers of atom occupancy n at each site of the optical lattice are observed as resonant atom losses. Here, the resonances corresponding to the singly occupied sites are identified from the spectra with the reduced atom number, and the corresponding resonance frequency is set to zero in Fig. 4.2 (upper). We also show a timing diagram for the spectroscopy in Fig. 4.3.

From the occupancy-resolved spectrum in Fig. 4.2 (upper), we can access the binding energies of the few-body quantum systems. In fact, as depicted in Fig. 4.2 (lower), the resonance frequency for each occupancy number n corresponds to the difference between the energies before and after the excitation of one atom from the ground state 1S_0 to the metastable excited state 3P_2 ($m_J = +2$). Here, we explicitly show the relation between the effective multi-body interaction energies entering the effective zero-dimensional Hamiltonian in Eq. (4.2) and the transition energies. The energies of $|g\rangle = \hat{b}_g^\dagger|0\rangle$, $|gg\rangle = (\hat{b}_g^{\dagger 2}/\sqrt{2!})|0\rangle$, $|ggg\rangle = (\hat{b}_g^{\dagger 3}/\sqrt{3!})|0\rangle$, $|gggg\rangle = (\hat{b}_g^{\dagger 4}/\sqrt{4!})|0\rangle$, $|ggggg\rangle = (\hat{b}_g^{\dagger 5}/\sqrt{5!})|0\rangle$, $|e\rangle = \hat{b}_e^\dagger|0\rangle$, $|eg\rangle = \hat{b}_e^\dagger\hat{b}_g^\dagger|0\rangle$, $|egg\rangle = (\hat{b}_e^\dagger\hat{b}_g^{\dagger 2}/\sqrt{2!})|0\rangle$, $|eggg\rangle = (\hat{b}_e^\dagger\hat{b}_g^{\dagger 3}/\sqrt{3!})|0\rangle$, $|egggg\rangle = (\hat{b}_e^\dagger\hat{b}_g^{\dagger 4}/\sqrt{4!})|0\rangle$ states are provided by

$$E_g = U_g, \quad (4.3)$$

$$E_{gg} = 2U_g + U_{gg}, \quad (4.4)$$

$$E_{ggg} = 3U_g + 3U_{gg} + U_{ggg}, \quad (4.5)$$

$$E_{gggg} = 4U_g + 6U_{gg} + 4U_{ggg} + U_{gggg}, \quad (4.6)$$

$$E_{ggggg} = 5U_g + 10U_{gg} + 10U_{ggg} + 5U_{gggg} + U_{ggggg}, \quad (4.7)$$

$$E_e = U_e, \quad (4.8)$$

$$E_{eg} = U_e + U_g + U_{eg}, \quad (4.9)$$

$$E_{egg} = U_e + 2U_g + 2U_{eg} + U_{gg} + U_{egg}, \quad (4.10)$$

$$E_{eggg} = U_e + 3U_g + 3U_{eg} + 3U_{gg} + 3U_{egg} + U_{ggg} + U_{eggg}, \quad (4.11)$$

$$E_{egggg} = U_e + 4U_g + 4U_{eg} + 6U_{gg} + 6U_{egg} + 4U_{ggg} + 4U_{eggg} + U_{gggg} + U_{egggg}. \quad (4.12)$$

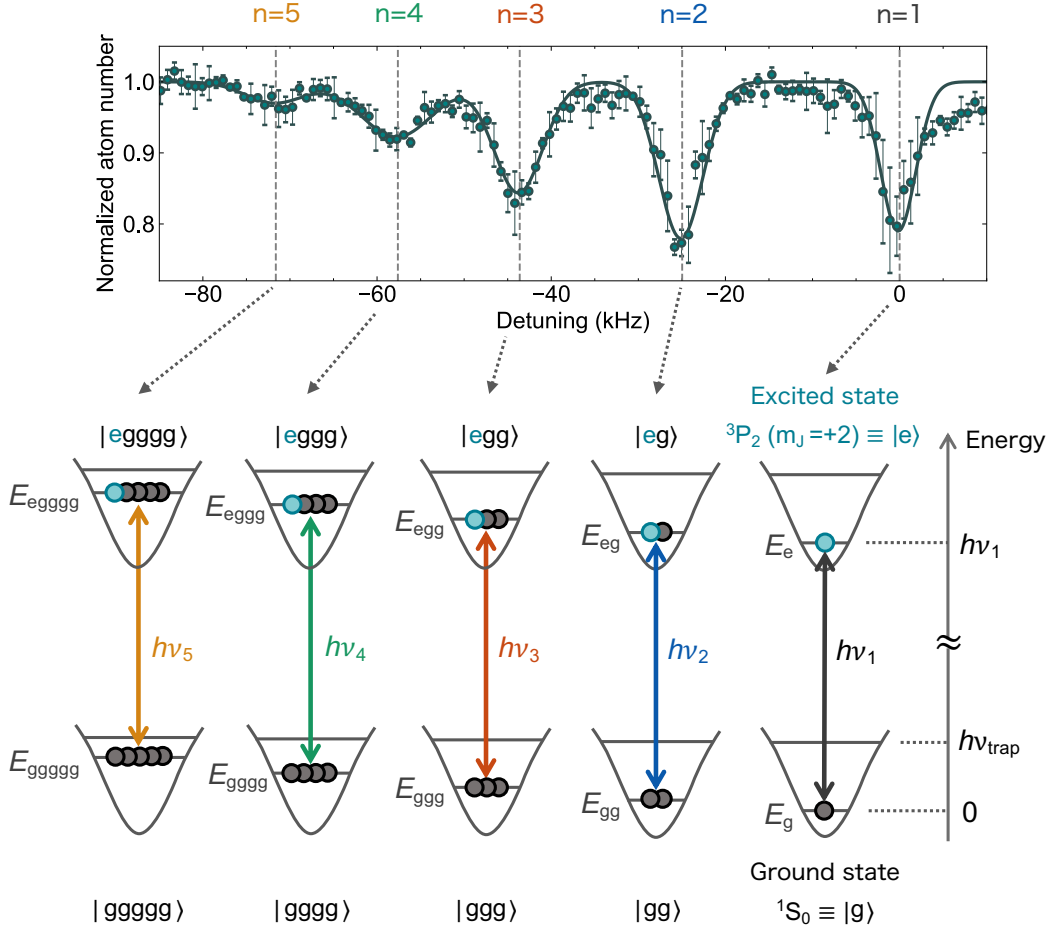


Figure 4.2: Occupancy-resolving spectroscopy of ^{174}Yb atoms in a three-dimensional optical lattice. (Upper) Typical spectroscopic result for the $^1S_0 \leftrightarrow ^3P_2 (m_J = +2)$ transition taken at a magnetic field strength of 232 mG, where the origin of the horizontal frequency axis is the resonance frequency of the singly occupied site. The error bars show the standard deviation of the four independent scans. The solid line denotes the result of the fit with the multi-Gaussian function. Note that the tail of $n = 1$ appears on the positive frequency side above about +5 kHz, which is considered to be derived from the excitation of center-of-mass motion for $n = 3$ sites (see also Sec. 4.2.1.2). The number of atoms corresponds to the number of ground-state atoms remaining in the crossed dipole trap after the lattice ramp-down sequence, normalized by the number of offset atoms in the fit result. The vertical dashed lines represent the resonance positions for the atom-filling, or occupancy of $n = 1, 2, \dots, 5$. (Lower) Schematic diagram of an isolated quantum few-body system realized at each site of an optical lattice. Before the laser excitation, the atoms are prepared in a few-body state $|gg \cdots g\rangle$ with the corresponding energy of $E_{gg \cdots g}$. By the laser excitation, only one of the atoms in the ground state is excited to the excited state due to the collision blockade effect, resulting in the few-body state of $|eg \cdots g\rangle$ with the energy $E_{eg \cdots g}$. The difference in the energies before and after the excitation $E_{eg \cdots g} - E_{gg \cdots g}$ corresponds to the resonance frequency ν_n for n -filling. The filling-dependent energy difference leads to a shift of the resonance position from the singly occupied resonance frequency ν_1 .

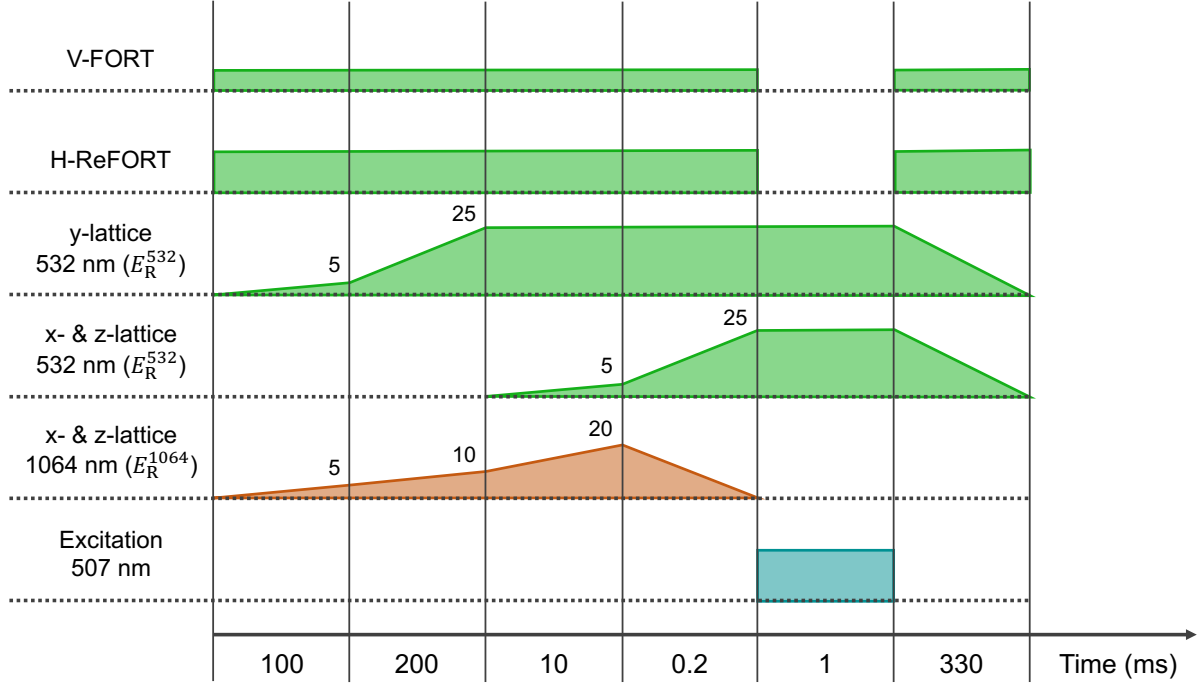


Figure 4.3: Timing diagram for the spectroscopy.

Therefore, the transition energies are found to be

$$h\nu_1 = E_e - E_g = U_e - U_g, \quad (4.13)$$

$$h\nu_2 = E_{eg} - E_{gg} = U_e - U_g + U_{eg} - U_{gg}, \quad (4.14)$$

$$\begin{aligned} h\nu_3 &= E_{egg} - E_{ggg} \\ &= U_e - U_g + 2U_{eg} - 2U_{gg} + U_{egg} - U_{ggg}, \end{aligned} \quad (4.15)$$

$$\begin{aligned} h\nu_4 &= E_{eggg} - E_{gggg} \\ &= U_e - U_g + 3U_{eg} - 3U_{gg} + 3U_{egg} - 3U_{ggg} \\ &\quad + U_{eggg} - U_{gggg}, \end{aligned} \quad (4.16)$$

$$\begin{aligned} h\nu_5 &= E_{egggg} - E_{ggggg} \\ &= U_e - U_g + 4U_{eg} - 4U_{gg} + 6U_{egg} - 6U_{ggg} \\ &\quad + 4U_{eggg} - 4U_{gggg} + U_{egggg} - U_{ggggg}, \end{aligned} \quad (4.17)$$

so that

$$h\nu_2 - h\nu_1 = U_{eg} - U_{gg}, \quad (4.18)$$

$$h\nu_3 - h\nu_1 = 2(h\nu_2 - h\nu_1) + U_{egg} - U_{ggg}, \quad (4.19)$$

$$h\nu_4 - h\nu_1 = 3(h\nu_3 - h\nu_2) + U_{eggg} - U_{gggg}, \quad (4.20)$$

$$h\nu_5 - h\nu_1 = 6(h\nu_3 - h\nu_1) - 8(h\nu_2 - h\nu_1) \\ + 4U_{eggg} - 4U_{gggg} + U_{egggg} - U_{ggggg} \quad (4.21)$$

$$= 4(h\nu_4 - h\nu_1) - 6(h\nu_3 - h\nu_1) + 4(h\nu_2 - h\nu_1) \\ + U_{egggg} - U_{ggggg}. \quad (4.22)$$

If the three-body and four-body interactions are neglected in Eqs. (4.19) and (4.20), we obtain Eqs. (4.28) in Sec. 4.3.3 and (4.30) in Sec. 4.3.4, respectively. Also, if the interactions with four and five bodies or more are neglected in Eqs. (4.21) and (4.22), we obtain Eqs. (4.32) and (4.33) in Sec. 4.3.4, respectively.

Below, we show the details of the data analysis of spectroscopic results. First, we determine the resonance position and its fitting error for every atomic occupancy n in each scan indexed as i by fitting the spectrum with a multi-Gaussian function given by

$$\sum_n a_{n,i} \exp \left[-\frac{(x - x_{n,i})^2}{2\sigma_n^2} \right] + b_i, \quad (4.23)$$

where x represents the laser frequency, $x_{n,i}$ the resonance position of the n occupancy, σ_n the width of the Gaussian function taken to be common to each scan, b_i the offset, and $a_{n,i}$ the amplitude of the Gaussian function. We perform this procedure for several, typically six, scans taken at the same magnetic field. Note that the quantity of interest in these measurements is not the absolute resonance position but the relative shift between the resonances. Thus, in the following, we consider $x_{\text{shift},n,i}$, the shift of the resonance frequency for n occupancy with respect to $n = 1$, given by $x_{\text{shift},n,i} = x_{n,i} - x_{n=1,i}$. Then, as a result of the fittings, we obtain $x_{\text{shift},n}$, a weighted average of the resonance position shifts, given as $x_{\text{shift},n} = \sum_i (w_{n,i} x_{\text{shift},n,i}) / \sum_i w_{n,i}$, using the weight $w_{n,i} = 1/\sigma_{\text{shift},n,i}^2$ where $\sigma_{\text{shift},n,i}$ is the fitting error.

We also obtain $\sigma_{n,\text{StdDev}}$, a weighted standard deviation of the resonance position shifts, given as $\sigma_{n,\text{StdDev}} = \sqrt{\sum_i [w_{n,i} (x_{\text{shift},n,i} - x_{\text{shift},n})^2] / \sum_i w_{n,i}}$, to represent the error of the resonance position shifts for every n at a certain magnetic field¹. In addition, the spectrum suffers from long-term laser frequency drifts, which also affect the relative frequency shifts. This effect is compensated for by a linear interpolation with the reference to the resonance position of $n = 2$ or $n = 1$. Here, we consider the difference between the resonance positions of $n = 1$ or $n = 2$ and the linear fit to them as the error σ_{Drift} of the drift compensation. Namely, $\sigma_{\text{Drift}} = \sqrt{\sum_i [w'_i (f_{\text{diff},i} - f_{\text{avg}})^2] / \sum_i w'_i}$, where $f_{\text{diff},i}$ is the frequency difference between the resonance positions of $n = 1$ or $n = 2$ and the linear fit to them in each scan indexed as i , f_{avg} is the average of $f_{\text{diff},i}$ weighted by the fitting errors $\sigma'_{\text{shift},n,i}$ of the resonance positions of $n = 1$ or $n = 2$, and $w'_i = 1/\sigma'^2_{\text{shift},n,i}$. Note that σ_{Drift} is typically about

¹The use of $\sigma_{n,\text{StdDev}}$ as a representative for the error is justified if $\sigma_{n,\text{StdDev}}$ is not much smaller than $\sigma_{n,\text{ErrProp}} = 1/\sqrt{\sum_i w_{n,i}}$ calculated from the fitting errors $\sigma_{\text{shift},n,i}$. However, this is not the case for the resonances of $n = 4$ and $n = 5$ at $B_0 = 232$ mG, $n = 3$ at 280 mG, and $n = 5$ at 327 mG, where we use $\sigma_{n,\text{ErrProp}}$ instead of $\sigma_{n,\text{StdDev}}$ to represent the error.

1.0–1.5 kHz. In the end, the value calculated with the following formula is used as the total error σ_{total} :

$$\sigma_{\text{total}} := \sqrt{\sigma_{n,\text{StdDev}}^2 + \sigma_{\text{Drift}}^2}. \quad (4.24)$$

We note that some of the $n = 1$ resonance spectra show a tail (see Fig. 4.2 (upper)), which is not represented by a simple Gaussian function. This additional structure is explained as the excitation of the center-of-mass motion for the $n = 3$ occupancy site, or $n = 2$, depending on the magnetic field strength. We estimate the associated error in the determination of the $n = 1$ resonance to be typically less than 0.3 kHz and not greater than 0.5 kHz. Since this is about two orders of magnitude smaller than the typical frequency shifts, we neglect this effect in the analysis.

4.3 Experimental Results

4.3.1 Variation of resonance-frequency shifts via a Feshbach resonance

In order to enter the strongly-interacting regime beyond the perturbative treatment of the interatomic interaction, we combine the inter-orbital Feshbach resonance with the occupancy-resolving high-resolution spectroscopy. Here, the scattering length a_{eg} between the ^{174}Yb atoms in the ground 1S_0 and excited 3P_2 ($m_J = +2$) states is controlled with a magnetic field via an anisotropy-induced Feshbach resonance [58]. Figures 4.4 and 4.5 show the measured frequency shift of the resonance position of the multiply occupied site with respect to the resonance frequency of the singly occupied site as a function of a magnetic field (Fig. 4.4) and the scattering length (Fig. 4.5). Here, the scattering length a_{eg} is determined from the $n = 2$ data using the interaction energy of two ground-state atoms $U_{gg} = 2\pi\hbar \times 4.04$ kHz, which is calculated for $\omega_g = 2\pi \times 35.9$ kHz and $a_{gg} = 5.55$ nm [190], and the following analytical formula [64], which relates the interatomic interaction U_{eg} and the scattering length a_{eg} :

$$\frac{1}{a_{eg}} \sqrt{\frac{\hbar}{m\omega_{eg}}} = \frac{\sqrt{2}\Gamma\left(-\frac{U_{eg}}{2\hbar\omega_{eg}}\right)}{\Gamma\left(-\frac{1}{2} - \frac{U_{eg}}{2\hbar\omega_{eg}}\right)}, \quad (4.25)$$

where $\Gamma(x)$ is the gamma function. Note that this analytical formula was derived for the special case of equal and isotropic trap frequency ω_{eg} for two atoms, which differs from our case of unequal and anisotropic trap frequencies. However, we find that the calculated U_{eg} using an average value of the trap frequencies ($\omega_{eg} = (1/3)\sum_{i=x,y,z}(\omega_{gi} + \omega_{ei})/2 = 2\pi \times 39.0$ kHz) is in close agreement with the numerical results, which fully take into account the unequal and anisotropic harmonic potentials for two atoms as in the experimental situation of this study. Because the relative difference is less than 1 %, we employ such approximation (equal frequency approximation) for the trap frequency to plot the theoretical curve in Figs. 4.4, 4.5, 4.7, and 4.8. Note that under the equal frequency approximation, the trap angular frequency in the presence of N atoms is given as follows: the trap angular

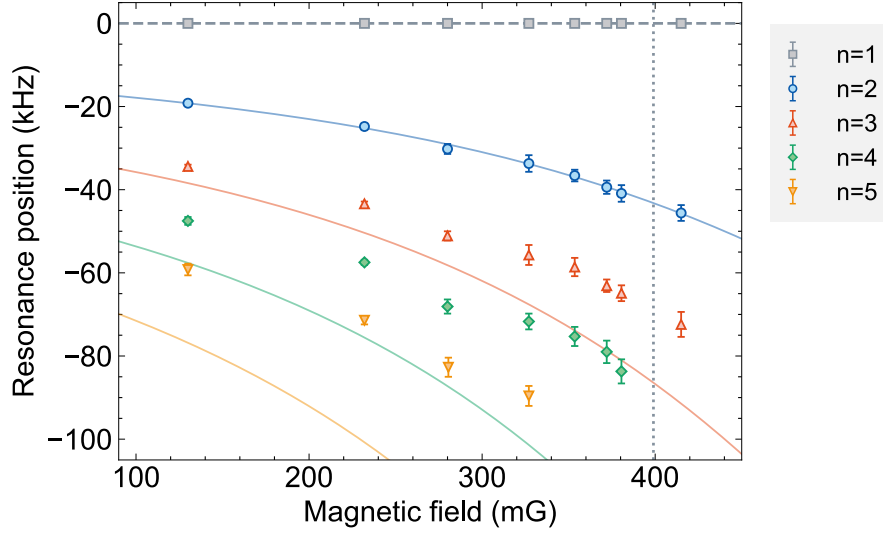


Figure 4.4: Variation of resonance positions for n -occupancy sites via a Feshbach resonance. Dependence on a magnetic field. The resonance positions corresponding to the $n = 1$ (gray square), $n = 2$ (blue circle), $n = 3$ (red triangle), $n = 4$ (green diamond), and $n = 5$ (orange inverted triangle) sites obtained from the spectra at each magnetic field strength are plotted. Note that the origin of the vertical frequency axis is taken as the resonance frequency of the single occupancy (horizontal dashed line). The error bars show the standard deviation of the resonance positions obtained from at least three independent scans, including errors associated with the correction for long-term laser frequency drift (see Sec. 4.2.1.2). The vertical dotted line denotes the Feshbach resonance point between $^1S_0 \leftrightarrow ^3P_2$ ($m_J = +2$) atoms at a magnetic field strength of 398 mG, obtained from the measured $n = 2$ resonance positions (see Fig. 4.6). Note that calibration of the magnetic field is done by observing the resonance position of $^1S_0 \leftrightarrow ^3P_2$ ($m_J = \pm 2$), and the accuracy of the magnetic field is about a few mG. The solid curves show calculated resonance positions including only the two-body interaction terms, where the solid curve at $n = 2$ (blue) shows a result of the theoretical calculation and the solid curves at $n = 3, 4$ and 5 (red, green, and orange) shows a result of the solid curve at $n = 2$ (blue) multiplied by 2, 3 and 4, respectively (see Sec. 4.2.1.2).

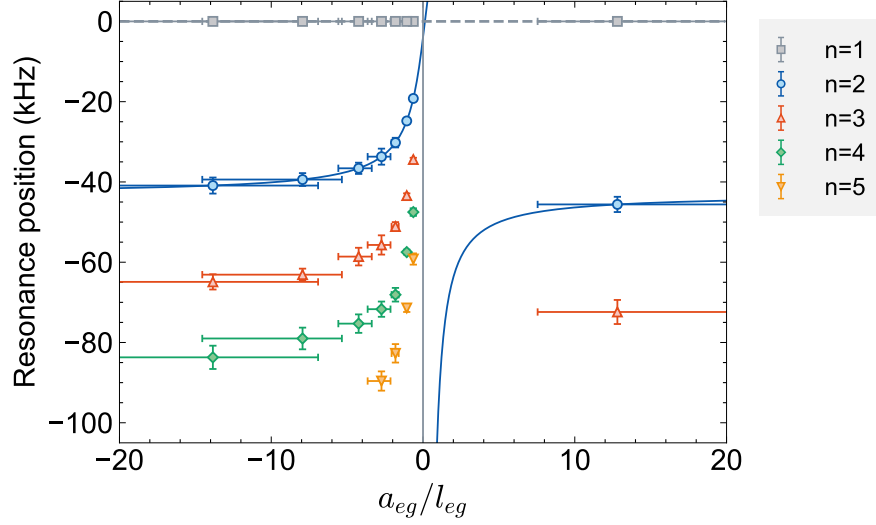


Figure 4.5: Variation of resonance positions for n -occupancy sites via a Feshbach resonance. Dependence on the scattering length a_{eg} . The horizontal axis represents the scattering length a_{eg} for atoms in the ground 1S_0 and excited 3P_2 ($m_J = +2$) states, divided by the harmonic oscillator length $l_{eg} = 39$ nm corresponding to the optical lattice depth of $25 E_R$. The blue solid curve at the $n = 2$ plots shows a result of the theoretical calculation. The horizontal error bars are evaluated for each field strength from the error in the determination of the scattering length.

frequency ω is set to be $\omega_g = 2\pi \times 35.9$ kHz if all N atoms are in the ground state, but it is assumed to be an average value of

$$\omega_{eg^{N-1}} = \frac{1}{3} \sum_{i=x,y,z} \frac{(N-1)\omega_{gi} + \omega_{ei}}{N} \quad (4.26)$$

$$= 2\pi \times \begin{cases} 39.0 \text{ kHz} & (N = 2) \\ 38.0 \text{ kHz} & (N = 3) \\ 37.5 \text{ kHz} & (N = 4) \end{cases} \quad (4.27)$$

if one of N atoms is excited. The corresponding harmonic oscillator lengths are denoted by $l_g = \sqrt{\hbar/(m\omega_g)}$ and $l_{eg^{N-1}} = \sqrt{\hbar/(m\omega_{eg^{N-1}})}$, respectively. The resulting magnetic field variation of a_{eg} is shown in Fig. 4.6². As the magnetic field approaches the value at the Feshbach resonance point indicated by the dotted line, the frequency shift also increases,

²The magnetic field strength at the Feshbach resonance point is obtained as $B_0 = 398(13)$ mG in this study, whereas that is $360(10)$ mG in the previous study [58]. We do not currently have a clear explanation for this discrepancy. Because the magnetic field is properly calibrated, as mentioned in Sec. 4.3, we describe the Feshbach resonance based on the present calibration of the magnetic field in this study.

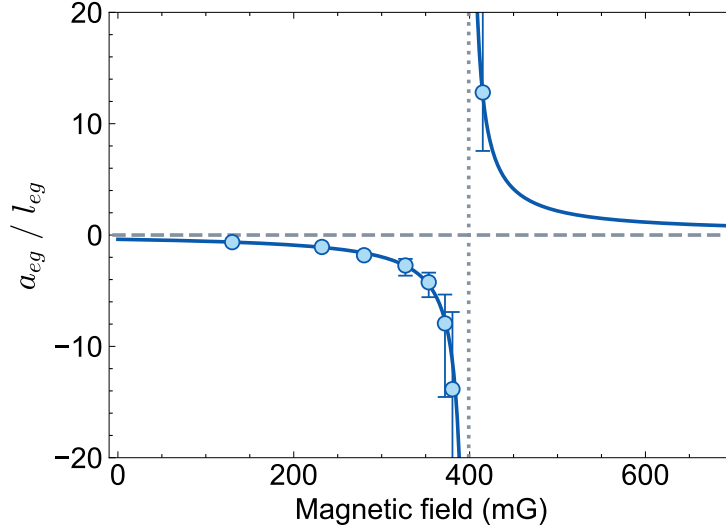


Figure 4.6: Magnetic field variation of the scattering length a_{eg} in the Feshbach resonance. The solid curve denotes a fit with a fitting function $a_{eg}(B) = a_{bg} - \Delta'/(B - B_0)$, with $a_{bg} = 0.13(0.16) l_{eg}$, $\Delta' = -206(45)$ mG, and $B_0 = 398(13)$ mG. The vertical error bars at each magnetic field strength are the same as the horizontal error bars in Fig. 4.5.

reflecting the larger absolute values of the scattering length a_{eg} . We also note that the resonance signals corresponding to the multiple occupancies, $n = 5$ in particular, become weaker around the Feshbach resonance, possibly due to the spectral broadening caused by the fast three-body inelastic loss of the atoms in the excited state.

The measured spectroscopic shifts for site occupations at a strongly-interacting regime clearly deviate from those expected within a two-body description (solid curves in Fig. 4.4). Note that strong non-linearity of interactions already manifests itself at the two-body level. In fact, the scattering lengths are determined by fitting the observed two-body resonances with the analytical formula given in Ref. [64].

Since the strong interactions are induced via the inter-orbital Feshbach resonance between $(n - 1)$ $|g\rangle$ -state bosons and a single $|e\rangle$ -state atom, rather than among n $|g\rangle$ -state bosons, the injected single $|e\rangle$ -state atom introduces the modification of the atomic wavefunctions of the relative motion between the $|e\rangle$ -state and other $|g\rangle$ -state atoms, resulting in the non-linearity of interactions. In addition, it is instructive to consider this injected few-body state in the context of the Bose polaron problem [191, 192] by regarding a single $|e\rangle$ -state atom as an impurity, which may provide another indispensable insight for this system.

4.3.2 Effective multi-body interactions in strongly-interacting regime

As an important example of encapsulating the strong interactions of a confined few-body system, we illustrate the novel behaviors of effective multi-body interactions. While the

emergence of effective multi-body interactions has already been corroborated in both theoretical and experimental works (e.g. Refs. [61], [55], and [60]), as is mentioned in the introductory section, the manner in which strong interactions involve not only modified two-body effective terms but also effective multi-body interactions is by no means trivial. In fact, the study of the effective multi-body interaction in the strongly-interacting regime was made possible by our experimental access to stronger interactions than those demonstrated so far by exploiting the inter-orbital Feshbach resonance.

4.3.3 Effective three-body interaction in strongly-interacting regime

We show the results for an effective three-body interaction in the strongly-interacting regime, which is beyond the perturbative treatment in previous works. Figure 4.7(a) shows the frequency shifts of $n = 2$ and $n = 3$ with respect to the resonance position of $n = 1$ in the $(\nu_2 - \nu_1, \nu_3 - \nu_1)$ plane. Here, in the presence of effective two-body interactions alone, the energy of the three-body system is obtained simply by pairwise interactions, and thus, a linear relationship of

$$\nu_3 - \nu_1 = 2(\nu_2 - \nu_1) \quad (4.28)$$

holds, which is shown as the dashed line in Fig. 4.7(a) (see Sec. 4.2.1.2). Clearly, we find a significant deviation between the experimental data and the dashed line, especially for the large scattering length region, corresponding to the lower left of the figure.

In order to quantitatively discuss the significance of the effective three-body interaction, we perform a chi-square test on the validity of Eq. (4.28), namely, the relation of $y = 2x$, where x and y represent the resonance frequency shifts of $n = 2$ and $n = 3$ from $n = 1$, respectively, by evaluating the χ^2 function defined as

$$\chi_{3\text{-body}}^2 := \sum_i \left[\left(\frac{x_i - \bar{x}_i}{\sigma_{\bar{x}_i}} \right)^2 + \left(\frac{2x_i - \bar{y}_i}{\sigma_{\bar{y}_i}} \right)^2 \right]. \quad (4.29)$$

Here, i is the index representing the data for each magnetic field, x_i are fitting parameters, and $(\bar{x}_i, \sigma_{\bar{x}_i})$ and $(\bar{y}_i, \sigma_{\bar{y}_i})$ are the measured resonance position shifts and their uncertainties for $n = 2$ and $n = 3$ from $n = 1$, respectively. In this χ^2 function, we search for the fitting parameters that minimize the sum of squares, and obtain the minimum value of $\chi_{3\text{-body},\min}^2 = 110$ (degree of freedom, $\text{dof} = 8$). This result corresponds to p -value = 3.33×10^{-20} , which corresponds to a significance of 9.2σ . In this way, we find the presence of the three-body interaction with such a large significance, owing to the Feshbach resonance control of the scattering length.

An interesting feature is found in the comparison of the experimental data with the perturbative calculations. The dashdot and solid curves in Fig. 4.7(a) show the results of perturbative calculations up to the second and third orders of the two-body interaction energy, respectively. Clearly, the second-order perturbation calculation does not reproduce any of the experimental data observed in our experiment on the one hand. The third-order

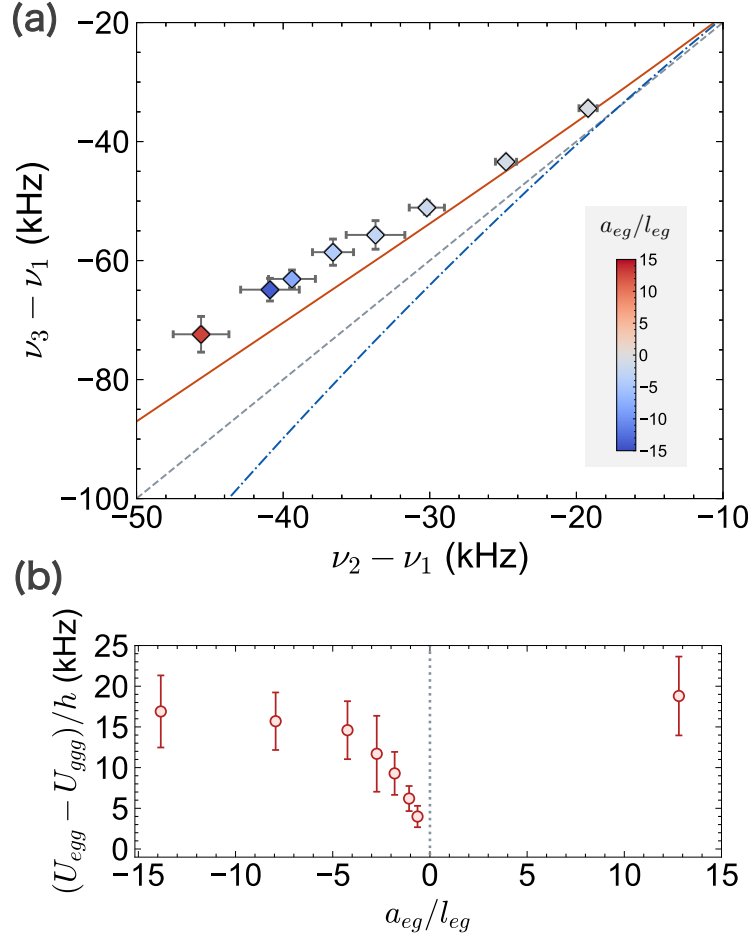


Figure 4.7: Effective three-body interaction in strongly-interacting regime. (a) Evidence of an effective three-body interaction in strongly-interacting regime obtained for the $n = 3$ resonance. The horizontal and vertical axes show the frequency shifts of $n = 2$ and $n = 3$ with respect to the resonance position of $n = 1$, respectively. The colorbar shows the scattering length a_{eg} divided by the harmonic oscillator length l_{eg} . The error bars for each axis are the same as those in Fig. 4.4. The dashed line represents a linear relation with slope 2, which holds between $\nu_3 - \nu_1$ and $\nu_2 - \nu_1$ when only the effective two-body interactions are incorporated, and the deviation from this line in the plots directly indicates the presence of effective three-body interactions. The dashdot and solid curves show the results of the perturbative calculations up to the second and third orders of the two-body interaction energy, respectively. (b) Amplitude of effective three-body interactions. Plotted here are values of $(U_{egg} - U_{ggg})/h = (\nu_3 - \nu_1) - 2(\nu_2 - \nu_1)$ (Eq. (4.19)) from measured resonance positions of $n = 2$ and 3. The error bars are calculated with the error propagation formula by using the error bars in Fig. 4.7(a).

result, on the other hand, can properly reproduce the data corresponding to the small scattering lengths where the perturbative calculation is justified. Note that the experimental data are all located on the upper side of the line of Eq. (4.28), which indicates the inequality $U_{egg} > U_{ggg}$ for the effective three-body interactions and the amplitude of the effective three-body interactions $U_{egg} - U_{ggg}$ is plotted in Fig. 4.7(b) as a function of a_{eg}/l_{eg} . This feature is properly captured by the perturbation calculation up to the third order, although the magnitudes of the deviations are not.

4.3.4 Evidence of effective four-body interaction

We provide an evidence regarding the presence of effective four-body interactions. Figure 4.8(a) shows the frequency difference between the resonance positions of $n = 2$ and $n = 3$, and that between $n = 1$ and $n = 4$ at each magnetic field, or scattering length in the $(\nu_3 - \nu_2, \nu_4 - \nu_1)$ plane. Here, in the absence of effective four-body interaction, it can be shown that a linear relationship of

$$\nu_4 - \nu_1 = 3(\nu_3 - \nu_2) \quad (4.30)$$

holds (see Sec. 4.2.1.2), which is indicated by the dashed line in Fig. 4.8(a). Therefore, the breakdown of this linearity is the smoking gun of the effective four-body interaction.

In Fig. 4.8(a), especially in the large scattering length region corresponding to the lower left of the figure, a significant deviation from the linear relationship is clearly seen, which is a direct evidence of effective four-body interaction. In order to quantitatively discuss the significance of the effective four-body interaction, we quantitatively evaluate the deviation from the linear relationship Eq. (4.30). Similar to the previous subsection, we perform a chi-square test on the validity of Eq. (4.30), namely, the relation of $z = 3\nu$, where z and ν represent the resonance frequency shift of $n = 4$ from $n = 1$ and that of $n = 3$ from $n = 2$, respectively, by evaluating the χ^2 function defined as

$$\chi_{4\text{-body}}^2 := \sum_i \left[\left(\frac{\nu_i - \bar{\nu}_i}{\sigma_{\bar{\nu}_i}} \right)^2 + \left(\frac{3\nu_i - \bar{z}_i}{\sigma_{\bar{z}_i}} \right)^2 \right]. \quad (4.31)$$

Here, ν_i are fitting parameters, $(\bar{\nu}_i, \sigma_{\bar{\nu}_i})$ and $(\bar{z}_i, \sigma_{\bar{z}_i})$ are the measured resonance positions and their uncertainties for $n = 3$ and $n = 4$ with respect to the resonance positions of $n = 2$ and $n = 1$, respectively, and the other symbols are the same as in Eq. (4.29). We obtain $\chi_{4\text{-body}, \min}^2 = 13.9$ (dof = 7) and p -value = 0.0534, which corresponds to a significance of 1.9σ . This result indicates that we successfully find a clear experimental evidence of the effective four-body interaction (see also Sec. 4.3.5).

Note that the plots are all located on the lower side of the line, which shows that the inequality $U_{eggg} < U_{gggg}$ holds for the effective four-body interactions, where U_{gggg} and U_{eggg} represent the interaction energy for the four atoms in the ground state $|g\rangle$ and that for three in the ground state and one in the excited state $|e\rangle$, respectively, and the amplitude of the effective four-body interactions $U_{eggg} - U_{gggg}$ is plotted in Fig. 4.8(b) as a function

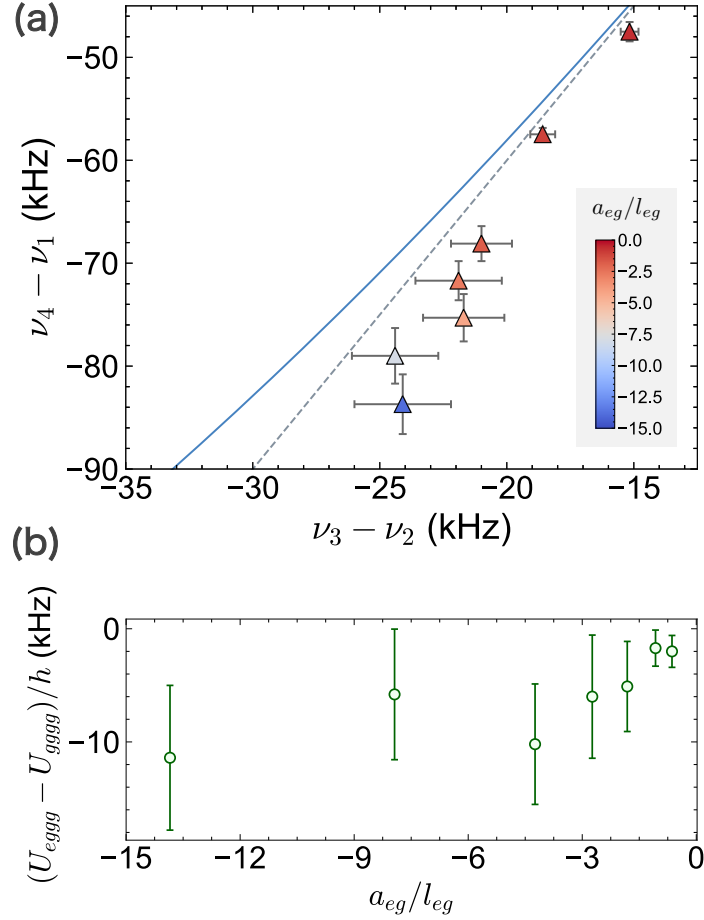


Figure 4.8: Evidence of an effective four-body interaction. (a) Evidence of an effective four-body interaction obtained for the $n = 4$ resonance. The horizontal and vertical axes represent the difference between the $n = 2$ and $n = 3$ resonance positions and that between $n = 1$ and $n = 4$, respectively. The colorbar shows the scattering length a_{eg} divided by the harmonic oscillator length l_{eg} . Error bars for the vertical axis are the same as those in Fig. 4.4, and error bars for the horizontal axis represent the standard deviation obtained in the analysis with respect to the resonance position of $n = 2$ (see Sec. 4.2.1.2). The dashed line represents a linear relation with slope 3, which holds between $\nu_4 - \nu_1$ and $\nu_3 - \nu_2$ when only up to effective three-body interactions are incorporated, and the deviation from this line in the plots is the direct evidence of the presence of effective four-body interactions. The solid curve shows the result of the perturbative calculation up to the third order of the two-body interaction energy. (b) Amplitude of effective four-body interactions. Plotted here are values of $(U_{eggg} - U_{gggg})/h = (\nu_4 - \nu_1) - 3(\nu_3 - \nu_2)$ (Eq. (4.20)) from measured resonance positions of $n = 2, 3$, and 4. The error bars are calculated by the error propagation formula using the error bars in (a).

of a_{eg}/l_{eg} . Since the Feshbach resonance is only induced between the atoms in the ground and excited states and not between the ground state atoms, U_{eggg} should be responsible for the emergence of the effective four-body interaction.

Figure 4.8(a) also shows as a solid curve the result of the perturbative calculation up to the third order of the two-body interaction energy, valid only in a region of relatively small scattering length. Clearly, the perturbative calculations do not reproduce the experimental data, including the direction of the deviation from the linear relationship Eq. (4.30), indicating the non-perturbative nature of the observed effective four-body interaction.

Furthermore, the experimental data of $n = 5$ resonance positions also support the presence of the effective four-body interaction. Figure 4.9 shows the measured $n = 5$ resonance positions with respect to that of $n = 1$ ($(\nu_5 - \nu_1)$, inverted triangles), the calculated $n = 5$ resonance positions including only effective two- and three-body interactions ($(\nu_5 - \nu_1)'$, circles), and the calculated $n = 5$ resonance positions including effective two-, three-, and four-body interactions ($(\nu_5 - \nu_1)''$, squares). Here,

$$(\nu_5 - \nu_1)' = 6(\nu_3 - \nu_1) - 8(\nu_2 - \nu_1), \quad (4.32)$$

$$(\nu_5 - \nu_1)'' = 4(\nu_4 - \nu_1) - 6(\nu_3 - \nu_1) + 4(\nu_2 - \nu_1). \quad (4.33)$$

See Sec. 4.2.1.2 for the derivation. To elucidate the contribution of the effective four-body interaction in the binding energy of the $n = 5$ sites, we perform a chi-square test. The χ^2 functions are defined as

$$(\chi_{4\text{-body}}^2)' := \sum_i \left[\left(\frac{x_i - \bar{x}_i}{\sigma_{\bar{x}_i}} \right)^2 + \left(\frac{y_i - \bar{y}_i}{\sigma_{\bar{y}_i}} \right)^2 + \left(\frac{6y_i - 8x_i - \bar{w}_i}{\sigma_{\bar{w}_i}} \right)^2 \right] \quad (4.34)$$

for testing the validity of Eq. (4.32), which holds in the absence of effective four-body interactions, and as

$$(\chi_{4\text{-body}}^2)'' := \sum_i \left[\left(\frac{x_i - \bar{x}_i}{\sigma_{\bar{x}_i}} \right)^2 + \left(\frac{y_i - \bar{y}_i}{\sigma_{\bar{y}_i}} \right)^2 + \left(\frac{z_i - \bar{z}_i}{\sigma_{\bar{z}_i}} \right)^2 + \left(\frac{4z_i - 6y_i + 4x_i - \bar{w}_i}{\sigma_{\bar{w}_i}} \right)^2 \right] \quad (4.35)$$

for testing the validity of Eq. (4.33), which holds in the presence of the effective four-body interactions. Here, x_i , y_i , and z_i are fitting parameters, $(\bar{w}_i, \sigma_{\bar{w}_i})$ are the measured resonance position shifts and their uncertainties for $n = 5$ from $n = 1$, and the other symbols are the same as in Eqs. (4.29) and (4.31). Note that we do not consider effective five-body interactions in both cases, and $6y_i - 8x_i$ in the third term of Eq. (4.34) and $4z_i - 6y_i + 4x_i$ in the fourth term of Eq. (4.35) reflect Eqs. (4.32) and (4.33), respectively. In these χ^2 functions, we obtain $(\chi_{4\text{-body}}^2)'_{\min} = 6.71$ (dof = 4) and $(\chi_{4\text{-body}}^2)''_{\min} = 0.46$ (dof = 4), which correspond to the p -values of 0.152 and 0.977, respectively. This analysis indicates that the measured $n = 5$ resonance positions are explained more plausibly by the presence of the effective four-body interaction.

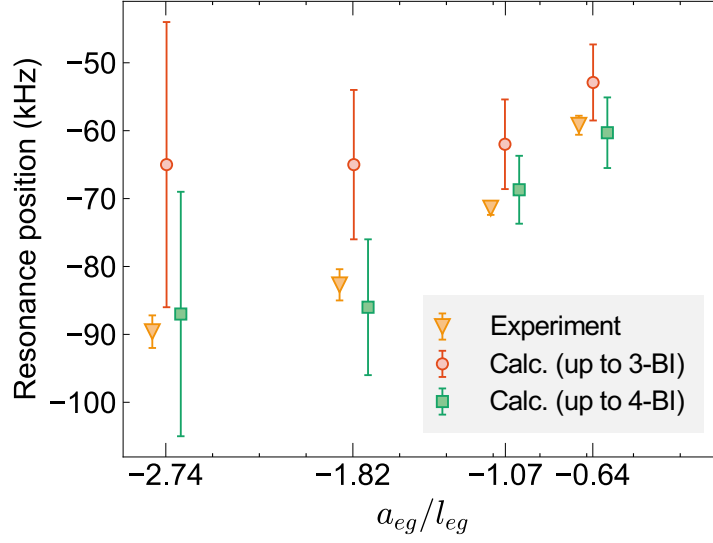


Figure 4.9: Contribution of effective four-body interactions to the $n = 5$ resonance. Plotted here are the measured $n = 5$ resonance positions (orange inverted triangles), the calculated $n = 5$ resonance positions by incorporating only up to effective three-body interactions (3-BI, red circles), and the calculated $n = 5$ resonance positions by incorporating up to effective four-body interactions (4-BI, green squares). Note that the plots at each scattering length are slightly shifted horizontally to avoid the overlap of the symbols. The error bars for the measured $n = 5$ resonance positions are the same as the error bars in Fig. 4.4, and the error bars in the calculated values are obtained with the error propagation formula by using the error bars for $n = 2, 3$, and 4 resonance positions.

4.3.5 Revisiting the results in previous studies

Finally, we revisit the experimental results in previous studies in which the effects of four-body interaction can appear, and see that these results can be explained by considering up to effective three-body interactions.

4.3.5.1 Chi-square analysis of the data in S. Will *et al.* (2010) [55]

In this previous study of performing time-resolved observations of quantum phase collapse and revival, the measured effective four-body interaction strength U_4 at each optical lattice potential depth is shown in Fig. 3b of that paper. Here, we read the values of U_4 and its errors from the figure and perform a chi-square test with the χ^2 function defined below, assuming that U_4 takes zero:

$$\chi^2 := \sum_i \left(\frac{\bar{y}_i}{\sigma_{\bar{y}_i}} \right)^2, \quad (4.36)$$

where i is the data index and $(\bar{y}_i, \sigma_{\bar{y}_i})$ are the measured quantities and their uncertainties for U_4 . In this χ^2 function, we obtain $\chi^2 = 1.72$ (dof = 5) and p -value = 0.886, which corresponds to a significance of 0.14σ . This indicates that U_4 is consistent with zero.

4.3.5.2 G. K. Campbell *et al.* (2006) [57]

In this previous study of imaging Mott insulators in a three-dimensional optical lattice with microwave spectroscopy, the measured dependence of the resonance position on the atomic occupation number n is shown in Fig. 2B (circle symbols) of that paper up to $n = 5$. The resonance positions corresponding to each n are read from the figure (no readings are available for error bars) and checked to see if the relationships of Eqs. (4.30) and (4.32), valid in the case of no effective four- and five-body interactions, are satisfied. As a result, the left- and right-hand sides of Eq. (4.30) are -88 Hz and -87 Hz, respectively, and the left- and right-hand sides of Eq. (4.32) are -111 Hz and -112 Hz, respectively. This means that both $n = 4$ and $n = 5$ shifts in this previous study can be explained by considering only up to effective three-body interactions.

4.3.5.3 A. Goban *et al.* (2018) [60]

In this previous study of performing high-resolution clock spectroscopy for fermionic ^{87}Sr atoms in a three-dimensional optical lattice, the measured dependence of the resonance position up to the atomic occupation number $n = 5$ is shown in Fig. 3 (red circles) of that paper. Here, the authors find that the measured values deviate from the calculated values when only two-body interactions are considered, while they are consistent with the perturbative calculation results that consider up to effective three-body interactions. They also mention in the supplementary information that the contribution of effective four-body interactions in their system is so small that they can be ignored, and in Fig. S1 the measured resonance positions up to $n = 5$ in the wide range of mean trap depths show ‘good agreement’ with the calculated values considering up to the effective three-body interactions.

4.3.5.4 L. Franchi *et al.* (2017) [59]

In this previous study of measuring the scattering properties of ultracold ^{174}Yb bosons with high-resolution spectroscopy in a three-dimensional optical lattice, the measured dependence of the resonance positions for doubly ($n = 2$, red circles) and triply ($n = 3$, blue circles) occupied sites on the potential depth of the 3D lattice is shown in Fig. 3 of that paper. Here, only up to the effective three-body interactions appear at most, and the authors find that the observed resonance positions show ‘very good agreement’ with the fit, which includes the effective three-body interactions calculated by the perturbation theory.

4.4 Summary and outlook

In this work, we reveal the behaviors of strongly-interacting few-body quantum systems comprising of harmonically confined spinless bosons in a wide range of bare two-body interactions with a high-resolution spectroscopy. Strong interactions are induced between the $(n - 1)$ $|g\rangle$ -state bosons and a single $|e\rangle$ -state atom, created as a result of the high-resolution laser excitation. It is thus instructive to consider this injected few-body state in the context of the Bose polaron problem, which may provide an indispensable viewpoint for this system. It is straightforward to apply the same methodology to study strongly-interacting regime of spinful atoms of both fermions and bosons, and also with long-range dipolar interactions provided by magnetic atoms and molecules or Rydberg atoms. Systematic investigations of these various systems would provide important insights into, for example, how the few-body limit can illuminate the quantum many-body problem by taking larger values of the number of atoms, which may provide a possible relation to a strongly-interacting bosonic liquid.

OBSERVATION OF THE SIGN REVERSAL OF THE MAGNETIC CORRELATION IN A DRIVEN-DISSIPATIVE FERMİ GAS IN DOUBLE WELLS

In this chapter, we report an experimental study of quantum magnetism in a dissipative Fermi gas. Especially, we observe a sign reversal of the magnetic correlation from antiferromagnetic to ferromagnetic in double wells, utilizing the dissipation caused by on-site two-body losses in a controlled manner. We first briefly summarize the theoretical background of the quantum magnetism in the dissipative Fermi-Hubbard model in a strongly correlated regime in Sec. 5.1. In Sec. 5.2, we describe the sample preparation and a photoassociation technique, which is utilized to introduce on-site two-body losses in a controlled manner. In Sec. 5.3, we describe the singlet-triplet oscillation (STO) method. Then, in Sec. 5.4-Sec. 5.6, we show the experimental results of systematic measurements of the nearest-neighbor spin correlation in an isolated double-well optical lattice, as well as a crossover from an isolated double-well lattice to a one-dimensional uniform lattice.

5.1 Theoretical background

In this section, we briefly summarize the theoretical background of the quantum magnetism in the dissipative Fermi-Hubbard model in a strongly correlated regime, based on Ref. [84].

We consider a dissipative Hubbard model with two-component fermions. Here, the unitary part of the dynamics is governed by the following Fermi-Hubbard Hamiltonian:

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma=\uparrow, \downarrow} \left(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right) + U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}, \quad (5.1)$$

where $\hat{c}_{i\sigma}$ is the fermionic annihilation operator for a site i and spin σ ; $\hat{n}_{j\sigma} = \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma}$ is the number operator; $t(>0)$ is the tunneling amplitude; and $U(>0)$ is the on-site interaction strength. The dissipative dynamics of the density matrix $\hat{\rho}$ of the system at time τ , where on-site two-body losses can occur, is described by the following quantum master equation [193]:

$$\frac{d\hat{\rho}}{d\tau} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + \frac{1}{2} \sum_{j,\sigma \neq \sigma'} \left(\hat{L}_{j\sigma\sigma'} \hat{\rho} \hat{L}_{j\sigma\sigma'}^\dagger - \frac{1}{2} \{ \hat{L}_{j\sigma\sigma'}^\dagger \hat{L}_{j\sigma\sigma'}, \hat{\rho} \} \right), \quad (5.2)$$

where $\hat{L}_{j\sigma\sigma'} = \sqrt{2\gamma} \hat{c}_{j\sigma} \hat{c}_{j\sigma'}^\dagger \delta_{\sigma,\uparrow} \delta_{\sigma',\downarrow}$ is the Lindblad operator, which describes the on-site two-body loss with the loss rate γ . In the following, we consider a strongly correlated regime and assume that a Mott-insulating state with unit filling is realized at the initial state. In this case, the Fermi-Hubbard model reduces to the following antiferromagnetic Heisenberg model:

$$\hat{H}_{\text{spin}} = J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right), \quad (5.3)$$

where $\mathbf{S}_i$ is the spin-1/2 operator; and $J = 4t^2/U$ is the spin-exchange interaction.

To investigate the dynamics described by Eq. (5.2), we employ the quantum trajectory method [67]. In this method, the dynamics is decomposed into two parts: a nonunitary Schrödinger evolution under an effective non-Hermitian Hamiltonian $\hat{H}_{\text{eff}} = \hat{H} - (i/2) \sum_{i,\sigma,\sigma'} \hat{L}_{i,\sigma,\sigma'}^\dagger \hat{L}_{i,\sigma,\sigma'}$ and stochastic quantum-jump processes which induce particle losses with the jump operators $\hat{L}_{j\sigma\sigma'}$. Here, we consider a trajectory that does not involve any loss event. This trajectory is governed by the following effective spin Hamiltonian:

$$\hat{H}_{\text{eff}} = (J_{\text{eff}} + i\Gamma) \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right), \quad (5.4)$$

where $J_{\text{eff}} = 4Ut^2/(U^2 + \gamma^2)$ and $\Gamma = 4\gamma t^2/(U^2 + \gamma^2)$. Note that Eq. (5.4) can be obtained by replacing the Hubbard interaction U with the inelastic interaction $U - i\gamma$ in Eq. (5.3). The eigenenergy of the Hamiltonian $\hat{H}_{\text{eff}}$ is given by $E_n = (J_{\text{eff}} + i\Gamma)E_n^{(0)}/J$, where $E_n^{(0)} \leq 0$ is the eigenenergy of the Heisenberg Hamiltonian in Eq. (5.3). From this, we find that the decay rate of the n -th eigenstate, Γ_n , which is given by the imaginary part of the energy, is proportional to $E_n^{(0)}$ as follows: $\Gamma_n = -\text{Im}[E_n] = -(\Gamma/J)E_n^{(0)} \geq 0$. Since $E_n^{(0)} \leq 0$, this indicates that the lower-energy state decays faster, i.e., has a shorter lifetime. For instance, considering the two-site case, a singlet state $(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)/\sqrt{2}$ with energy $E_0^{(0)} = -J$ has a shorter lifetime than a triplet state $(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle)/\sqrt{2}$ with energy $E_1^{(0)} = 0$, and this is due to a possible loss in an intermediate state involving a double occupancy as a second-order process, which can occur only in the singlet state (see also Fig. 5.1). Therefore, only the high-energy states survive in the long-time limit. From this, it is expected that an initial antiferromagnetic ensemble of the two-site system, where there are more singlet states than triplet states, changes to a ferromagnetic one during the dissipative dynamics (see Fig. 5.1).

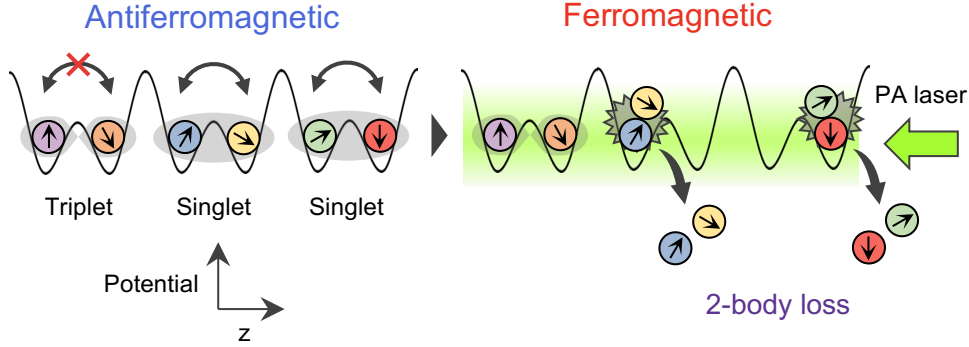


Figure 5.1: Schematic illustration of the mechanism of the reversal of the magnetic correlation from the antiferromagnetic (left) to the ferromagnetic correlation (right) in dissipative double wells with on-site two-body losses. Here, we show the case of six spin-components (magnetic quantum number $m_F = -5/2, -3/2, \dots, +5/2$) in the system, which is the same situation as in this study. While double occupancy on the same site occurs in the singlet state, which has a spatially symmetric wave function, it is prohibited by the Pauli exclusion principle in the triplet state, which has a spatially antisymmetric wave function. Thus, only singlet states are lost under on-site two-body losses, which makes the nearest-neighbor magnetic correlation reverse. In this work, we induce on-site two-body losses with a PA process. Figure adapted from Ref. [194].

5.2 Experimental setup

5.2.1 Sample preparation

A degenerate Fermi gas of six-component ^{173}Yb ($T/T_F \sim 0.15$, T_F : Fermi temperature), which is generated by evaporative cooling, is loaded into an optical superlattice which realizes a dimerized or a 1D optical lattice as well as the crossover between them. Our optical lattice potential is given by

$$V(x, y, z) = -V_{\text{short}}^{(z)} \cos^2(2k_L z + \pi/2) - V_{\text{long}}^{(z)} \cos^2(k_L z) - V_{\text{short}}^{(x)} \cos^2(2k_L x) - V_{\text{short}}^{(y)} \cos^2(2k_L y), \quad (5.5)$$

where $k_L = 2\pi/\lambda$ with $\lambda = 1064$ nm is the wave number of the long lattice ($V_{\text{long}}^{(z)} = 0$ for a 1D uniform optical lattice). In the following, we represent the potential depth of the optical lattice as $s_L = [s_{\text{short}}^{(x)}, s_{\text{short}}^{(y)}, (s_{\text{short}}^{(z)}, s_{\text{long}}^{(z)})] = [V_{\text{short}}^{(x)}, V_{\text{short}}^{(y)}, (V_{\text{short}}^{(z)}, V_{\text{long}}^{(z)})]/E_R$, where $E_R = \hbar^2 k_L^2 / 2m$ is the recoil energy for the long lattice. This system is described by the Fermi-Hubbard model in a dimerized lattice, where the corresponding Hamiltonian is given as follows:

$$\hat{H} = -t_d \sum_{\langle i,j \rangle, z, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) + \frac{U}{2} \sum_{j, \sigma \neq \sigma'} \hat{n}_{j\sigma} \hat{n}_{j\sigma'} - \mu \sum_{j, \sigma} \hat{n}_{j\sigma}$$

$$-t \sum_{\langle i,j \rangle_z, \sigma} \left(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right) - t_{xy} \sum_{\langle i,j \rangle_{xy}, \sigma} \left(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right), \quad (5.6)$$

where $\hat{c}_{i\sigma}$ is the fermionic annihilation operator for a site i and spin σ ; $\hat{n}_{j\sigma} = \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma}$ is the number operator; t_d , t , and t_{xy} are the tunneling amplitudes between nearest-neighbor sites in the intra-dimer bond $\langle i, j \rangle_z$, the inter-dimer bond $\langle i, j \rangle_z$ along the z -axis, and the inter-dimer bond $\langle i, j \rangle_{xy}$ along the $x(y)$ -axis, respectively; U is the on-site interaction strength; and μ is the chemical potential.

Typical parameters for the optical superlattice are $s_L = [80, 80, (20.8, 20)]$, and the corresponding Hubbard parameters are $t_d/h = 1.0$ kHz, $U/t_d = 4.0$, $t/h = 38$ Hz, and $t_{xy}/h = 10$ Hz. Here, the tunneling amplitudes along the dimerized lattice are determined by fitting a tight-binding model to the energy bands obtained from the first principle calculation for the superlattice potential. For the on-site interaction strength, we constructed the Wannier function with the method described in Sec. 2.2.4.3.

5.2.2 Photoassociation technique

In this work, we introduce on-site two-body losses as dissipation utilizing a PA technique. In the PA process, two ground-state atoms in a doubly occupied site where a PA laser beam is irradiated are converted to an electronically excited short-lived molecule, which rapidly escapes from an optical trap [195, 79, 196, 197]. In this way, on-site two-body losses are realized with the PA laser, enabling us to control the dissipation strength by controlling the PA laser intensity.

To induce on-site two-body losses as dissipation, we apply the PA laser, which is detuned by -5.76 GHz from the $^1S_0 \leftrightarrow ^3P_1$ ($F' = 7/2$) transition. We measure the on-site two-body loss rate due to the PA laser in an isolated double-well lattice of $s_L = (80, 80, (20.8, 20))$, into which evaporatively cooled six-component ^{173}Yb atoms are loaded. Here, different from the case of the spin correlation measurement, we load a sufficient number of atoms to prepare doubly occupied sites. In Fig. 5.2, we show the results of the loss rate measurement and a typically observed atom loss dynamics (inset). Here, we fit the data with a double exponential function, where the initial faster decay corresponds to the on-site two-body loss, and the later slower decay corresponds to the one-body loss mainly due to the photon scattering. As shown in Fig. 5.2, we observe the saturation of loss rate γ_{PA} at a large intensity of the PA laser, which has also been observed in previous works [79, 198, 199, 200, 201], and we only use the PA intensities in the unsaturated regime. Note that the PA light does not play a role in one-body losses or the heating effect due to the use of the deep PA resonance, far detuned by -5.76 GHz from the $^1S_0 \leftrightarrow ^3P_1$ ($F' = 7/2$) transition. Since the photon-scattering rate for atoms of single occupation at intensity ~ 20 W/cm² is calculated to be $\gamma_{\text{photon}} = 0.021$ /ms, it is ensured that the effect of photon scattering is negligible in the time scale that we measure the dynamics in this work (< 2 ms). Here, the photon scattering rate

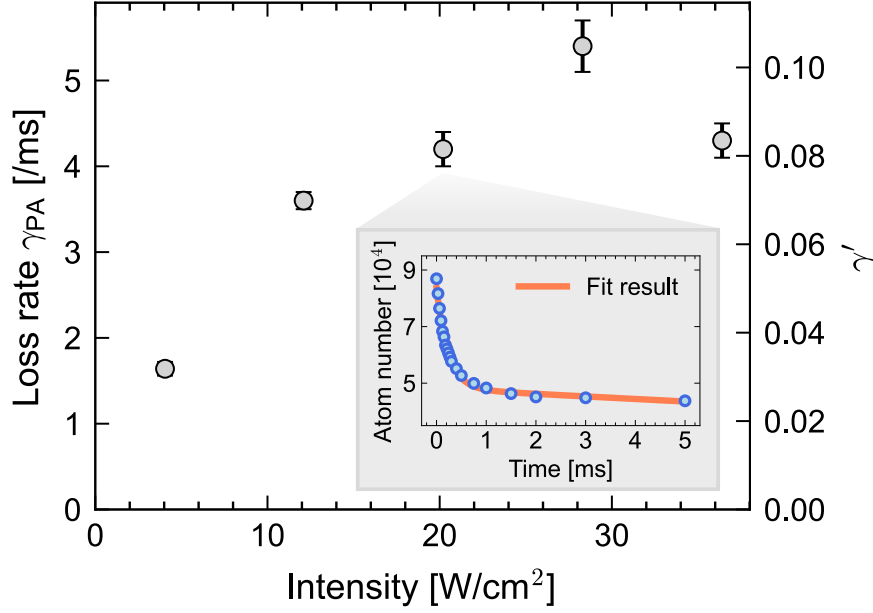


Figure 5.2: Two-body loss rate γ_{PA} due to the PA laser. Here, we show the dependency of the loss rate γ_{PA} (dimensionless dissipation strength γ' in the right axis) on the intensity of the PA laser. Error bars denote the fitting error to the atom loss dynamics. The inset shows the typical observed atom loss dynamics, where the orange solid curve shows the fit result by a double exponential function. Error bars denote the standard deviation of three independent scans (smaller than the plots). Figure adapted from Ref. [194].

γ_{photon} is given as follows:

$$\gamma_{\text{photon}} = \frac{3\pi c^2 \omega^3 I}{2\hbar} \sum_i \left[\frac{\Gamma_i}{\omega_i^3} \left(\frac{1}{\omega - \omega_i} + \frac{1}{\omega + \omega_i} \right) \right]^2, \quad (5.7)$$

where ω is the angular frequency of the laser; I is the intensity of the laser; and c is the velocity of the light. The summation is taken over all possible transitions i from the state in which the atom is; and ω_i and Γ_i are the resonant angular frequency and the linewidth for each transition i , respectively. We also note that we confirm that the PA line for dissipation is active for all spin pairs in six-component ^{173}Yb gases, as shown in Fig. 5.3(a). Here, we prepare various two spin-component mixtures by performing an optical pumping to a six-component ^{173}Yb gas at the initial stage of evaporative cooling (see Ref. [149] for the details of the experimental setup for the optical pumping). A slight spin-pair dependence of the PA rate observed within the experimental uncertainty is not evident in observed STO signals, and therefore, in this work, we analyze the data by assuming no spin-pair dependence and using Eq. (5.13), as described later.

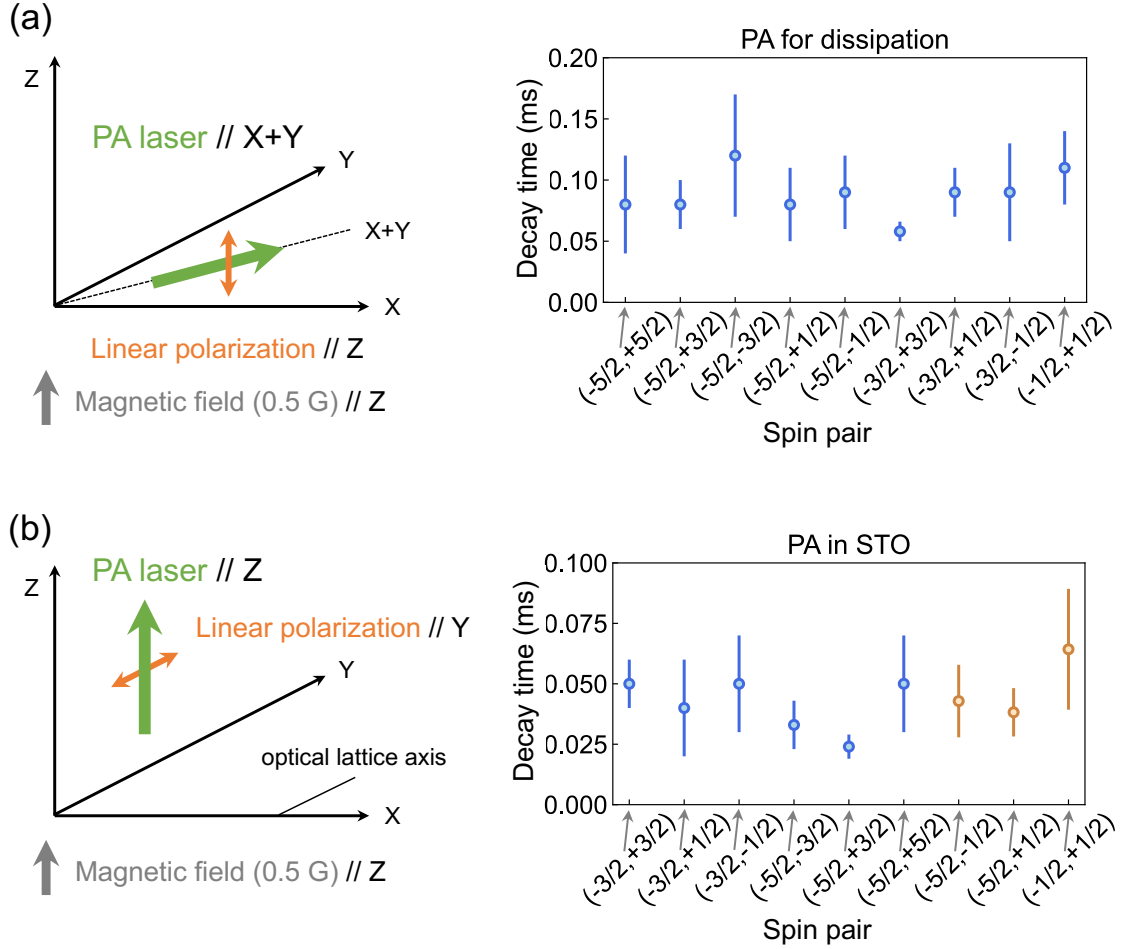


Figure 5.3: Dependency of PA loss rates on spin-pairs of a six-component ^{173}Yb gas. (a) PA for dissipation. (left) Experimental configuration for PA experiment for dissipation. (right) Results of atom loss measurements with a PA laser in a 532 nm 3D optical lattice. Note that although the number of possible spin pairs in six spin components is ${}_6C_2 = 15$, it is enough to examine the action of the PA laser on the 9 pairs shown in (a)(right) considering the symmetry. (b) PA for the STO method. (left) Experimental configuration for PA experiment for the STO method. (right) Results of atom loss measurements with a PA laser in a 532 nm 3D optical lattice. Here, the dark orange plots correspond to the previously obtained data (in Ref. [196]) as a reference.

5.3 Single-triplet oscillation method

5.3.1 Derivation of the expressions of STO amplitude A and singlet/triplet fraction p_s/p_{t_0}

In this section, we derive the expressions of STO amplitude A and singlet (triplet) fraction p_s (p_{t_0}). First, we derive an expression of the STO signal for the case of two spins (σ_1, σ_2) in a dimer described by the Heisenberg model. If a spin-dependent potential at a dimer induces an energy difference $\Delta = \hbar\omega$ (ω : STO frequency) between the states $|\sigma_1, \sigma_2\rangle$ and $|\sigma_2, \sigma_1\rangle$, the time evolution of the state initially in the singlet state $|s\rangle = (|\sigma_1, \sigma_2\rangle - |\sigma_2, \sigma_1\rangle)/\sqrt{2}$ and that of the state initially in the triplet state $|t_0\rangle = (|\sigma_1, \sigma_2\rangle + |\sigma_2, \sigma_1\rangle)/\sqrt{2}$ are as follows:

$$\begin{pmatrix} |s(t)\rangle \\ |t_0(t)\rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} |\sigma_1, \sigma_2\rangle - e^{-i\omega t} |\sigma_2, \sigma_1\rangle \\ |\sigma_1, \sigma_2\rangle + e^{-i\omega t} |\sigma_2, \sigma_1\rangle \end{pmatrix} = \begin{pmatrix} \cos \frac{\omega t}{2} |s\rangle - i \sin \frac{\omega t}{2} |t_0\rangle \\ \sin \frac{\omega t}{2} |s\rangle + i \cos \frac{\omega t}{2} |t_0\rangle \end{pmatrix}. \quad (5.8)$$

Here, if the probabilities of being in the singlet state and the triplet state at $t = 0$ are P_s, P_{t_0} respectively, the probability of observing the singlet state after the time evolution by time t is given from Eq. (5.8) by

$$\begin{aligned} P_s(t) &= \text{Tr}[\rho(t) |s\rangle \langle s|] = P_s |\langle s|s(t)\rangle|^2 + P_{t_0} |\langle s|t_0(t)\rangle|^2 \\ &= \frac{P_s + P_{t_0}}{2} + \frac{P_s - P_{t_0}}{2} \cos(\omega t), \end{aligned} \quad (5.9)$$

where $\rho(t) = P_s |s(t)\rangle \langle s(t)| + P_{t_0} |t_0(t)\rangle \langle t_0(t)|$ is the density operator at time t . In the STO measurement sequence, we first drive STOs in probed dimers, remove singlet states selectively with the PA laser, and perform the absorption imaging (see Sec. 5.3.2). Thus, the atom number dynamics $N_{\text{STO}}(t)$ (STO signal) observed after the STO measurement sequence is given from Eq. (5.9) by

$$\begin{aligned} N_{\text{STO}}(t) &= N - N_s(t) = N[1 - P_s(t)] \\ &= \left(N - \frac{N_s + N_{t_0}}{2} \right) - \frac{N_s - N_{t_0}}{2} \cos(\omega t), \end{aligned} \quad (5.10)$$

where N is the total atom number and $N_s = NP_s$ ($N_{t_0} = NP_{t_0}$) is the number of atoms being initially in the singlet (triplet) state.

This expression of the STO signal for the case of two spin components is generalized to the case of $\mathcal{N}(> 2)$ spin components. In this case, $\mathcal{N}C_2$ (number of possible spin pairs)

different STO frequencies generally appear in the STO signal and the form of the STO signal is given by

$$N_{\text{STO}}(t) = N - \sum_{(\alpha,\beta)} \left[\frac{N_s^{\alpha\beta} + N_{t_0}^{\alpha\beta}}{2} + \frac{N_s^{\alpha\beta} - N_{t_0}^{\alpha\beta}}{2} \cos(\omega_{\alpha\beta} t) \right], \quad (5.11)$$

where $N_s^{\alpha\beta}, N_{t_0}^{\alpha\beta}$ are the atom numbers being initially the singlet state and the triplet state of spin pair (α, β) respectively, and $\omega_{\alpha\beta}$ is the STO frequency for the spin pair (α, β) . In our STO measurement sequence, $\mathcal{N} = 6$ and only three STO frequencies $\omega_1, \omega_2, \omega_3$ (each for four spin pairs) with a simple relation $\omega_1 : \omega_2 : \omega_3 = 1 : 2 : 3$ appear (see Sec. 5.3.2). With this fact and the assumption of $\text{SU}(\mathcal{N})$ symmetry in the spin correlation, namely, that all possible spin combinations equally contribute to the spin correlation (i.e., $N_s^{\alpha\beta} = N_s / \mathcal{N} C_2$ and $N_{t_0}^{\alpha\beta} = N_{t_0} / \mathcal{N} C_2$), the STO signal is given from Eq. (5.11) by

$$N_{\text{STO}}(t) = -c \frac{N_s - N_{t_0}}{2} \frac{1}{3} [\cos(\omega t) + \cos(2\omega t) + \cos(3\omega t)] + \left[N - \frac{N_s + N_{t_0}}{2} - (1 - c) \frac{N_s - N_{t_0}}{2} \right], \quad (5.12)$$

where ω is the smallest STO frequency; and $c = 12/15 = 4/5$ is the fraction of spin pairs in which STO occurs out of the possible spin pairs. This form of the STO signal leads to the fitting function to the experimentally obtained data:

$$f(t) = -\frac{a}{3} e^{-t/\tau} [\cos(\omega t) + \cos(2\omega t) + \cos(3\omega t)] + b. \quad (5.13)$$

To quantify the spin correlation, we use the normalized STO amplitude $A = c(N_s - N_{t_0})/N_{\text{tot}}$, the singlet fraction $p_s = N_s/N_{\text{tot}}$, and the triplet fraction $p_{t_0} = N_{t_0}/N_{\text{tot}}$, which are normalized by the total atom number N_{tot} in the lattice with no PA laser for dissipation. By comparing corresponding terms in Eq. (5.12) (N : the total atom number in the lattice after the irradiation of the PA laser for dissipation) with those in Eq. (5.13), we obtain the expressions of A , p_s , and p_{t_0} with the fitting parameters a and b :

$$A = (4/5)(N_s - N_{t_0})/N_{\text{tot}} = 2a/N_{\text{tot}}, \quad (5.14)$$

$$p_s = N_s/N_{\text{tot}} = (N + a - b)/N_{\text{tot}}, \quad (5.15)$$

$$p_{t_0} = N_{t_0}/N_{\text{tot}} = (2N - 3a - 2b)/2N_{\text{tot}}. \quad (5.16)$$

5.3.2 Experimental sequence for observing the STO signal

The typical sequence of the STO measurement is as follows (see Fig. 5.4). Note that we call a probed dimer the specific neighboring sites for measuring the spin correlation.

(1) Tunneling freezing: we freeze tunneling between intra- and inter- dimer sites by ramping up the long lattice depth of double wells to $s_L = (80, 80, (20.8, 25))$ in 0.5 ms, followed by ramping up the short lattice depth to $s_L = (80, 80, (80, 25))$ in 10 ms. We note that

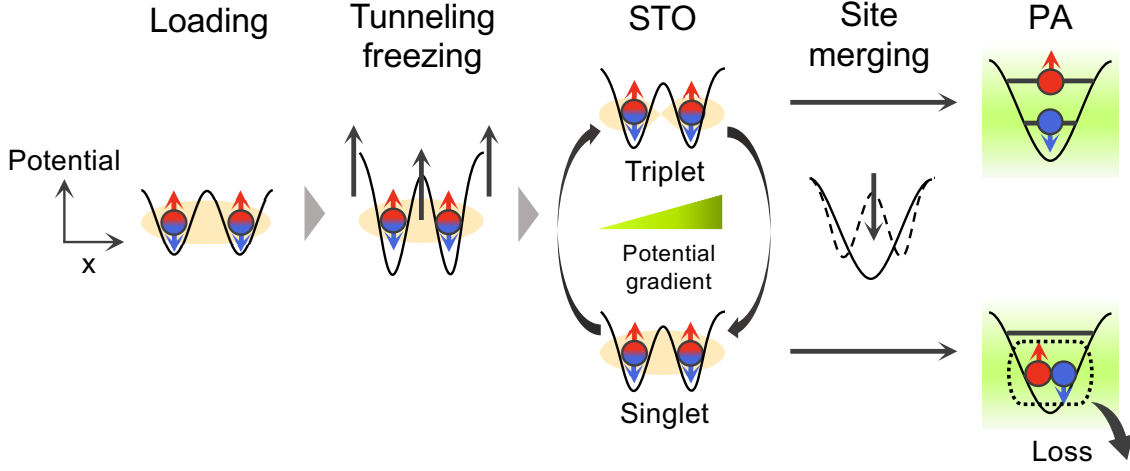


Figure 5.4: Schematic illustration of the sequence for STO measurement in a dimer. Here, we show the case of two spins (red and blue) per dimer. The sequence flows as loading, tunneling freezing, STO, site merging, and PA. Depending on the STO time, the two spins form the state in which one spin occupies the lowest band and the other spin occupies the first excited band, or the state in which both spins occupy the lowest band. Atoms in the latter state are removed by the PA laser. Figure adapted from Ref. [194].

the adiabaticity of this ramp-up sequence is confirmed by numerical calculation (Supplemental Material of Ref. [196]).

(2) STO: we drive STOs in probed dimers by irradiating a gradient beam, which induces a spin-dependent potential gradient for atoms. This potential gradient creates an energy difference Δ for atoms with different spins in a probed dimer, and the spin states in the dimer coherently oscillate between the singlet state $|s\rangle = (|\sigma_1, \sigma_2\rangle - |\sigma_1, \sigma_2\rangle)/\sqrt{2}$ and the triplet state $|t_0\rangle = (|\sigma_1, \sigma_2\rangle + |\sigma_1, \sigma_2\rangle)/\sqrt{2}$ at a frequency $\Delta/\hbar$ (STO frequency), where $\sigma_i (i = 1, 2)$ denotes a spin component. In this work, we use a linearly polarized light with 2.7 GHz blue detuning from the $^1S_0 \leftrightarrow ^3P_1$ ($F' = 7/2$) transition as the gradient beam, which makes the differential light shift the same for the spin pairs of $(|m_F| = 1/2, 3/2)$ with the corresponding STO frequency ω_1 , $(3/2, 5/2)$ with ω_2 , and $(1/2, 5/2)$ with ω_3 . Note that an STO does not occur for the spin pairs with the same $|m_F|$, namely, $(m_F = -1/2, 1/2)$, $(-3/2, 3/2)$, and $(-5/2, 5/2)$ because the differential light shifts are zero for these spin pairs. In addition to this, a simple relation $\omega_1 : \omega_2 : \omega_3 = 1 : 2 : 3$ holds between these frequencies due to the properties of the Clebsch-Gordan coefficients for the associated transition (see Sec. 3.6.1). Note that this relation is independent of the detuning of the gradient beam. We also note that actually observed STO signals suffer from decoherence mainly due to the spatial inhomogeneity of the gradient beam. This effect is taken into account in an exponential decay term in the fitting function (see Eq. (5.13)).

(3) Site merging: we ramp down the short lattice depth to $s_L = (80, 80, (0, 25))$ in 1 ms. Here, two atoms in the singlet state which has a spatially symmetric two-particle wave function both occupy the lowest band, while for two atoms in the triplet state which has

a spatially antisymmetric two-particle wave function, one atom occupies the lowest band and the other atom occupies the first excited band.

(4) Irradiation of the PA laser: we irradiate the PA laser and remove two atoms that doubly occupy the lowest band, corresponding to the detection of the singlet states. The PA laser in the STO sequence is detuned by -812 MHz from the $^1S_0 \leftrightarrow ^3P_1$ ($F' = 7/2$) transition [196, 197]. Note that we confirm that the PA line for the STO is active for all spin pairs, as shown in Fig. 5.3(b). After irradiating the PA laser, the absorption imaging follows, in which observed atom number dynamics reflects the magnetic correlation of the prepared sample.

We note that, instead of measuring the atom number of each spin component, the number of singlet pairs N_s and triplet pairs N_{t_0} are calculated from Eqs. (5.15) and (5.16) through fitting the data with Eq. (5.13) under the assumption of SU(6) symmetry, namely, that all possible spin pairs equally contribute to the spin correlation. Note that the correspondence between the sign of the slope of STO signals at initial time and the spin correlation can be understood by the correspondence between the coefficient a in the fitting function Eq. (5.13) and the STO amplitude A in Eq. (5.14).

5.4 Dynamical reversal of the magnetic correlation in an isolated double-well lattice

To reveal the effects of the on-site two-body loss on the magnetic correlation, we first measure the spin correlation dynamics in a dissipative isolated double-well lattice. Figures 5.5(a), 5.5(b), and 5.5(c) show the results of the normalized STO amplitude A , the singlet fraction p_s , and the triplet fraction p_{t_0} , respectively. We also show a typical timing diagram for this measurement in Fig. 5.6. The STO data are taken for the atom number $N_{\text{tot}} = 2.7 \times 10^4$, which is small enough to suppress double occupancies. Dimensionless dissipation strength $\gamma' = \hbar\gamma/U = \hbar(\gamma_{\text{PA}}/2)/U$ is 0.082(4), where γ_{PA} is the two-body loss rate due to the PA laser ($\gamma_{\text{PA}} = 4.2(2)$ /ms) and is measured from atom loss dynamics in an isolated double-well lattice (see Sec. 5.2.2). We note that while γ and γ_{PA} are tunable via the PA laser power and detuning as well as the lattice depth, γ' does not depend on the lattice depth. In this measurement, the dependency of the spin correlation dynamics on the magnitude of initial ($t_{\text{PA}} = 0$) antiferromagnetic correlations is also investigated, which is realized by changing atom-loading schemes into an isolated double-well lattice. Here, we prepare three systems with different initial antiferromagnetic (AFM) conditions (i), (ii), and (iii) in Fig. 5.5, as follows (see Fig. 5.7):

- (i) Large AFM condition (normalized STO amplitude $A \sim 0.3$).

Load to isolated double-well lattices along z -axis, which has a lattice depth of $s_L = (80, 80, (20.8, 20))$, from the beginning.

- (ii) Medium AFM condition ($A \sim 0.2$)

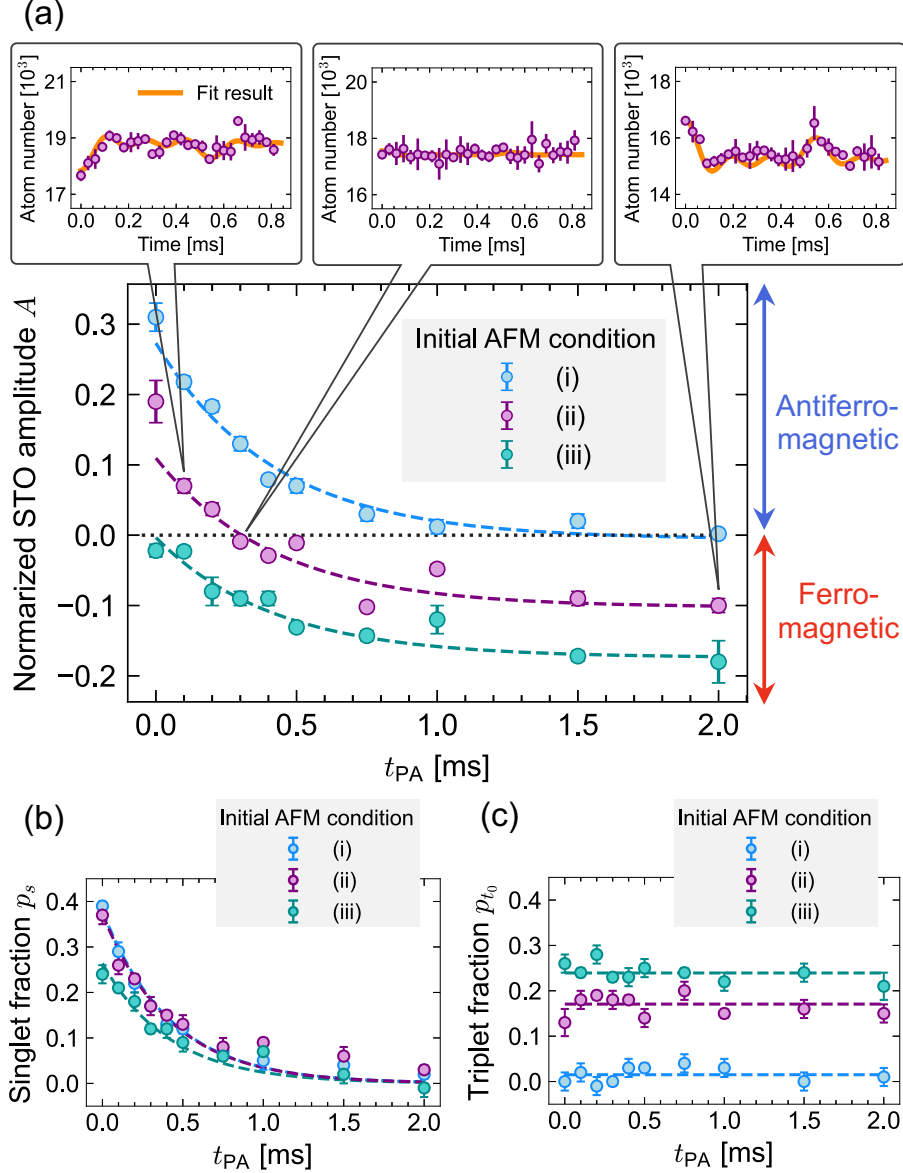


Figure 5.5: Dynamics of (a) the normalized STO amplitude A , (b) the singlet fraction p_s , and (c) the triplet fraction p_{t_0} in an isolated double-well lattice with on-site two-body losses. Here, we show their dependency on the irradiation time t_{PA} of the PA laser. In (a), three different initial antiferromagnetic (AFM) conditions are prepared with different atom-loading schemes into an optical lattice. The dashed curves in (a), (b), and (c) show the results of the exponential fit of the data with an offset, without an offset, and the constant fit, respectively, where the damping time constant of the exponential function is determined by the co-fit to A and p_s . Error bars denote the standard deviation, which is calculated with fitting errors of STO measurement and the standard deviations of the total atom number. In markup balloons in (a) (upper), measured STO signals for the initial condition (ii) are shown, which correspond to $t_{PA} = 0.1$ ms, 0.3 ms, and 2.0 ms in order from the left. Error bars in STO signals denote the standard deviation of three scans. Figure adapted from Ref. [194].

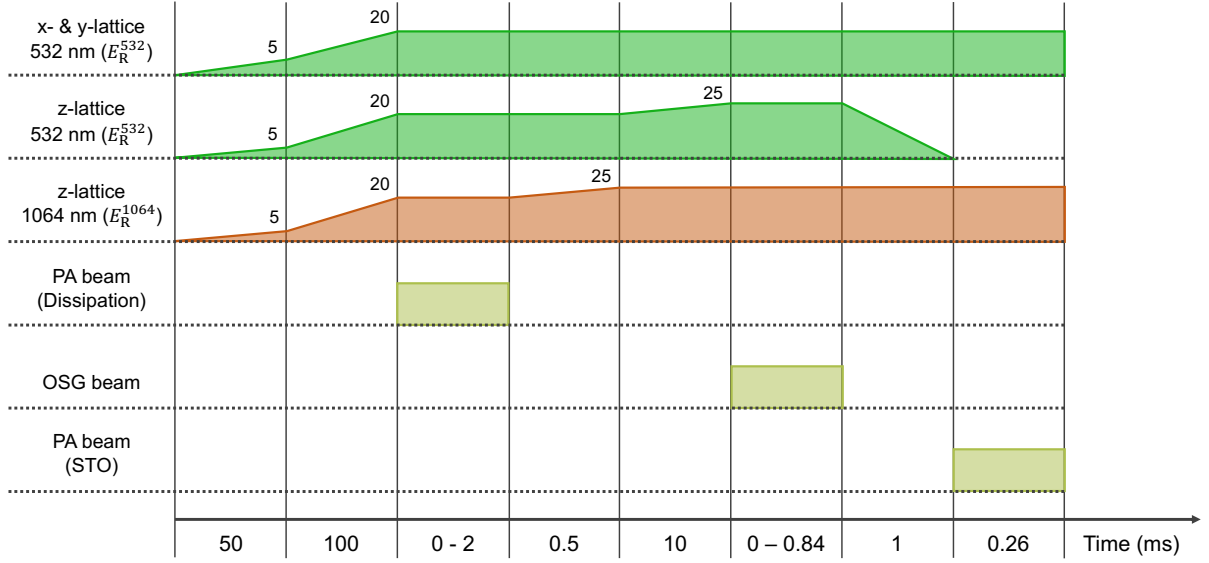


Figure 5.6: Typical timing diagram for the measurement of the spin correlation dynamics in a dissipative isolated double-well lattice. Here, we show the diagram for the case of the initial AFM condition (i).

First load to a three-dimensional lattice and switch to isolated double-well lattices along z -axis in 0.5 ms: $s_L = (28, 28, (28, 0)) \rightarrow (80, 80, (20.8, 20))$.

(iii) Small AFM condition ($A \gtrsim 0.0$)

First load to one-dimensional lattices along x -axis and switch to isolated double-well lattices along z -axis in 0.5 ms: $s_L = (19.8, 80, (80, 0)) \rightarrow (80, 80, (20.8, 20))$.

In Fig. 5.5(a), the normalized STO amplitude decreases as the dissipation is introduced, regardless of the initial conditions. Especially, in the initial condition (ii), the form of the STO signal reverses due to the dissipation, indicating the sign of A changing from positive to negative (Fig. 5.5: upper left to right). This means that the magnetic correlation between the nearest neighbor sites in the isolated double-well lattice changes from an antiferromagnetic to ferromagnetic correlation, which has been theoretically predicted [84]. Note that a state with sign-reversed magnetic correlation, where the population of triplet states is greater than that of singlet states, corresponds to the negative spin temperature state [202]. Here, we define the spin temperature T_{spin} as

$$\frac{p_{t_0}}{p_s} = \exp\left(-\frac{J}{k_B T_{\text{spin}}}\right), \quad (5.17)$$

where k_B is the Boltzmann constant; p_s/p_{t_0} is the singlet/triplet fraction; and J is the exchange interaction. In Fig. 5.8, we show the result of the dynamics of $1/T_{\text{spin}}$ measured in a dissipative isolated double-well lattice, which corresponds to the result for the initial AFM condition (ii) shown in Fig. 5.5. As dissipation is introduced, $1/T_{\text{spin}}$ reverses from positive

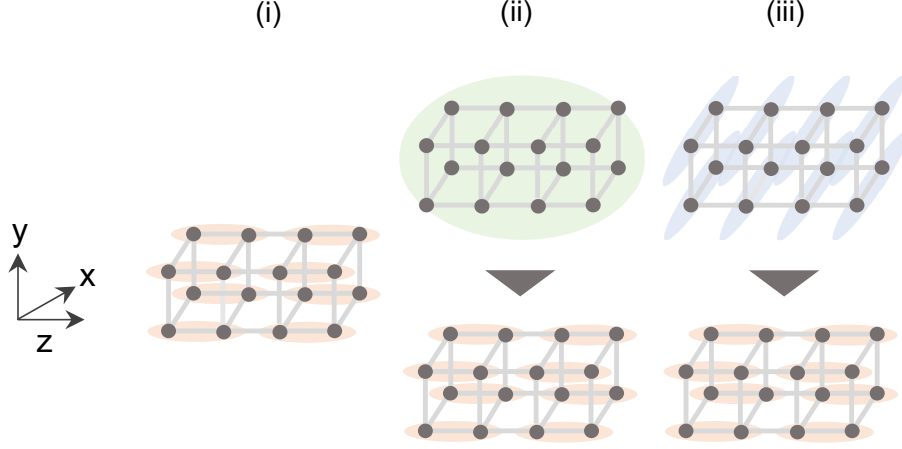


Figure 5.7: Schematic illustration of three different atom-loading schemes into isolated double-well lattices: (i) Load to isolated double-well lattices along z -axis from the beginning. (ii) First load to a three-dimensional lattice and switch to isolated double-well lattices along z -axis in 0.5 ms. (iii) First load to one-dimensional lattices along x -axis and switch to isolated double-well lattices along z -axis in 0.5 ms. Figure adapted from Ref. [194].

to negative via zero at which $p_s = p_{t_0}$. This result demonstrates that a negative temperature state, which has been realized in an isolated system [203], can also be realized in an open quantum system with dissipation. We also note that the photon scattering by the PA laser, which can decrease spin correlations, is negligible on the time scale of this measurement. Figure 5.5(b) shows that the singlet fraction p_s decreases by the application of the dissipation, while the triplet fraction p_{t_0} shows no apparent decrease, as shown in Fig. 5.5(c). These results are in good agreement with the theoretical consideration that the change of the spin correlation is solely due to the decrease of the number of the singlet state while that of the triplet state is kept constant. Note that the observed behaviors originating from two-body physics inside the double-well are common, irrespective of SU(2) or SU(6) system. The dissipative SU(6) system realized in this work opens the door for the study of non-ergodic dynamics in the dissipative SU($\mathcal{N}$) Fermi-Hubbard model [122].

5.5 Dependency of the dissipative dynamics on the dissipation strength and the exchange interaction

Next, we investigate the dependency of the spin correlation dynamics in an isolated double-well lattice on the dissipation strength γ' and the exchange interaction $J = 4t_d^2/U$. When $U \gg t_d$, the loss rate of the singlet state is theoretically given as $2\Gamma/\hbar$ where $\Gamma = J\gamma'/(1 + \gamma'^2)$ [84]. Considering $\gamma' \ll 1$ for this measurement, we expect the linear dependency of the decay rate of p_s on γ' and J . We note that the continuous Quantum Zeno effect, which sup-

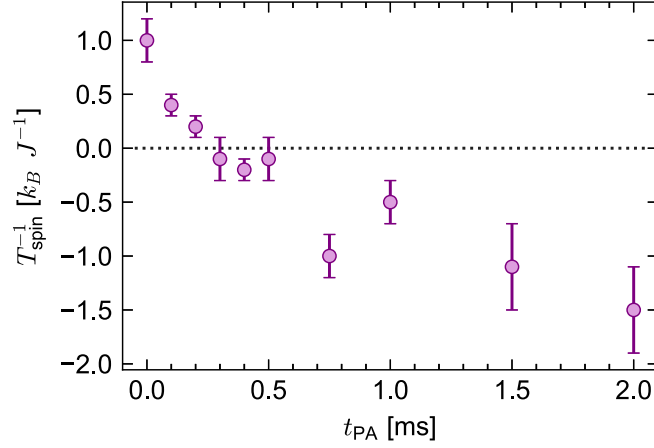


Figure 5.8: Dynamics of the inverse of the spin temperature T_{spin} calculated from the result for the initial AFM condition (ii) shown in Fig. 5.5(b) and 5.5(c). Here, we show the dependency of the inverse of T_{spin} on the irradiation time t_{PA} of the PA laser. Error bars denote the standard deviation, which is calculated from the standard deviations of p_s and p_{t_0} . Figure adapted from Ref. [194].

presses Γ at $\gamma' \gg 1$, does not play a role in this measurement with $\gamma' \ll 1$. Figure 5.9(a) (left) shows the result of the singlet fraction p_s measured at each dissipation strength γ' . One can clearly see that the larger the dissipation strength is, the faster p_s decays. In Fig. 5.9 (a) (right), we show the dependency of the decay rate of p_s on the dissipation strength γ' . We find that the decay rate of p_s increases approximately in proportion to γ' . The dotted line in Fig. 5.9(a) (right) represents the result of the calculation considering the finite value of $U/t_d = 4$ in our case, which also shows the linear dependence, similar to the experimental data.

In the calculation considering the finite value of U/t_d , we consider a two-site Fermi-Hubbard model with on-site two-body losses. There, we calculate the time evolution of the following ground state of the two-site Fermi-Hubbard Hamiltonian $\hat{H}$ (two-site case of Eq. (5.1)) using the non-Hermitian Hamiltonian $\hat{H}_{\text{eff}} = \hat{H} - (i/2) \sum_{i,\sigma,\sigma'} \hat{L}_{i,\sigma,\sigma'}^\dagger \hat{L}_{i,\sigma,\sigma'}$:

$$|\psi(0)\rangle = \frac{1}{\mathcal{N}} \left[\frac{4t_d}{-U + \sqrt{U^2 + 16t_d^2}} (|\sigma_1, \sigma_2\rangle - |\sigma_2, \sigma_1\rangle) + |0, \sigma_1 \sigma_2\rangle + |\sigma_1 \sigma_2, 0\rangle \right], \quad (5.18)$$

where $\mathcal{N}$ is a normalization factor that ensures $\langle \psi(0) | \psi(0) \rangle = 1$. In the dynamics under $\hat{H}_{\text{eff}}$, the squared norm of a state is not conserved due to non-Hermiticity. The squared norm, which is initially normalized to unity, corresponds to the probability of having no loss events during the dynamics [67]. Thus, the decay rate of the squared norm of the singlet state (5.18) corresponds to the decay rate of the singlet fraction p_s . Note that we found that

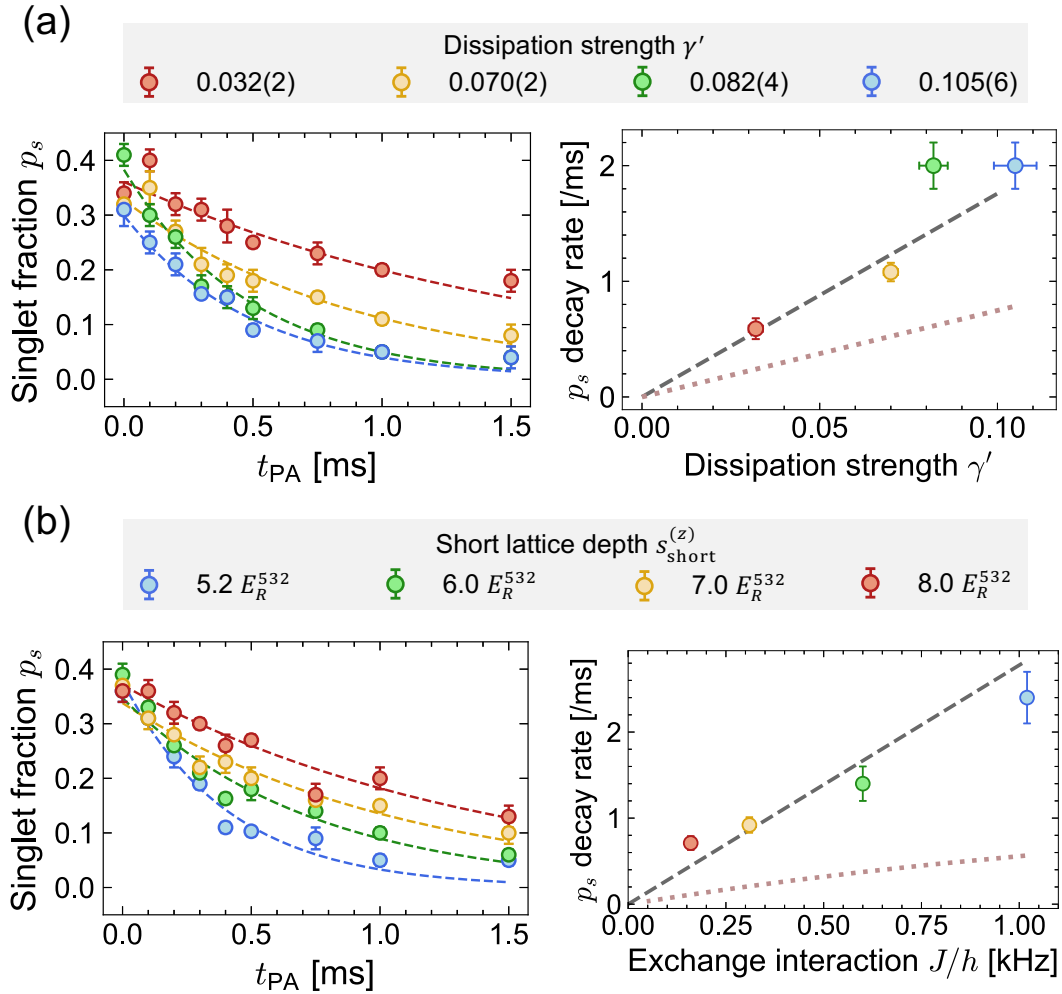


Figure 5.9: (a) (left) Dynamics of the singlet fraction p_s for each dissipation strength γ' in a dissipative isolated double-well lattice. Each dashed curve shows the results of the exponential fit without an offset. (right) Dependency of the decay rate of p_s obtained by the exponential fit on the dissipation strength γ' . The gray dashed line shows the result of the linear fit through the origin. The dotted line shows the result of the calculation considering the finite value of $U/t_d = 4$ in our case. Vertical error bars denote the fitting error of the exponential fit to p_s . Horizontal error bars denote the errors of the measured two-body loss rates. (b) (left) Dynamics of the singlet fraction p_s for each short lattice depth in a dissipative isolated double-well lattice. Here, E_R^{532} denotes the recoil energy of the short lattice. Each dashed line shows the results of the exponential fit without an offset. (right) Dependency of the decay rate of p_s obtained by the exponential fit on the exchange interaction J . The gray dashed line shows the result of the linear fit through the origin. The dotted line shows the result of the calculation considering the finite value of U/t_d . Figure adapted from Ref. [194].

the time evolution of the squared norm is approximated as

$$\langle \psi(t) | \psi(t) \rangle \simeq e^{-2\Gamma t/\hbar}, \quad (5.19)$$

and the singlet decay rate is given by $2\Gamma/\hbar$ with

$$\begin{aligned} \Gamma &= -\text{Im}[E_0] \\ &= \frac{1}{2} \left(\hbar\gamma - \sqrt{\frac{-x + \sqrt{x^2 + y^2}}{2}} \right), \end{aligned} \quad (5.20)$$

where $x := U^2 + 16t_d^2 - (\hbar\gamma)^2$ and $y := -2\hbar U\gamma$ (see the supplemental material of Ref. [194] for more details of the calculation, which was performed by Dr. Masaya Nakagawa).

Figure 5.9(b) (left) shows the result of the singlet fraction p_s measured at each short lattice depth, where the dissipation strength is fixed at $\gamma' = 0.082(4)$. The shallower the short lattice depth is, namely, the larger the magnitude of the exchange interaction J is, the faster p_s decays. We note that U/t_d changes from 4.0 to 10.9 when $s_{\text{short}}^{(z)}$ changes from 5.2 to 8.0. In Fig. 5.9(b) (right), we show the dependency of the decay rate of p_s on the exchange interaction J . We find that the decay rate of p_s increases approximately in proportion to J , which is qualitatively consistent with the calculated results showing approximate linear dependence of p_s on J . Note that we confirm that the singlet decay rate Γ is approximately proportional to J under the fixed dimensionless dissipation strength $\gamma' = \hbar\gamma/U$ even in the regime of $U \gtrsim t_d$. In Fig. 5.10, we show the dependence of

$$\frac{\Gamma}{\gamma'J} = \frac{1}{8} \left(\frac{U}{t_d} \right)^2 - \frac{1}{8\gamma'} \left(\frac{U}{t_d} \right)^2 \sqrt{\frac{-1 - 16(t_d/U)^2 + (\gamma')^2 + \sqrt{(1 + 16(t_d/U)^2 - (\gamma')^2)^2 + 4(\gamma')^2}}{2}} \quad (5.21)$$

on the short-lattice depth $s_{\text{short}}^{(z)}$. The dependency of $\Gamma/(\gamma'J)$ on $s_{\text{short}}^{(z)}$ is small (deviation/mean < 21%), meaning that the plots of the singlet decay rate p_s against J fall approximately on the same line.

We also note that the observed discrepancy in the values between the experimental data and theoretical calculation in Fig. 5.9 may be partially explained by a slight uncertainty in PA rates; Another PA-rate measurement in a deep 3D lattice configuration, which is a different lattice configuration in Fig. 5.2, and in which the inter-site hopping is negligible, gives a higher PA rate after the compensation for the difference in the spatial spread of the Wannier function.

5.6 Crossover from an isolated double-well lattice to a 1D uniform lattice

Finally, we measure spin correlations in the presence of the dissipation in a crossover from an isolated double-well lattice to a 1D uniform lattice. Figure 5.11(a) shows the result of

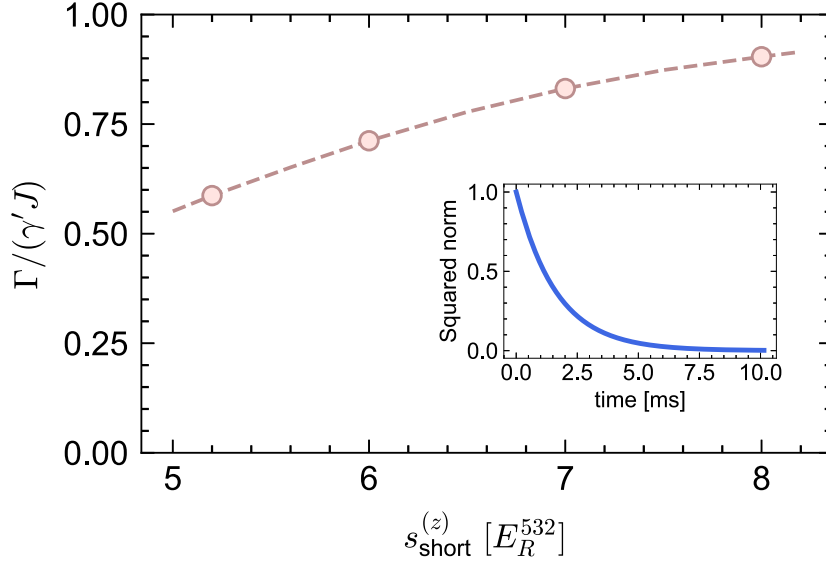


Figure 5.10: Dependency of $\Gamma/(\gamma'J)$ on the short-lattice depth. Here, Γ is half of the singlet decay rate times $\hbar$ calculated with Eq. (5.20); $\gamma' = \hbar\gamma/U$ is the dimensionless dissipation strength fixed to 0.082(4); and $J = 4t_d^2/U$ is the exchange interaction. The dots correspond to the values for $s_{\text{short}}^{(z)} = 5.2, 6.0, 7.0, 8.0$. The inset shows a typical result for the dynamics of the squared norm of the singlet state (Eq. (5.18)) under $\hat{H}_{\text{eff}}$ calculated with exact diagonalization for the parameters $U/t_d = 4.0$ and $\gamma' = 0.082$. Figure adapted from Ref. [194].

the dependency of the normalized STO amplitude A on the long lattice depth. Here, we prepare the sample in the initial condition corresponding to (iii) in Figs. 5.5 and 5.7, and therefore the initial spin correlation is expected to be almost zero or small antiferromagnetic one. In this measurement, the dissipation strength γ' is fixed to 0.082(4). We note that we restrict the irradiation time of the PA laser t_{PA} to 0.5 ms in this measurement to suppress the effect of hopping between 1D tubes and photon scattering by the PA laser. As shown in Fig. 5.11(a), we find that the formation of the ferromagnetic spin correlation is suppressed for the smaller long-lattice depths at which atoms can tunnel to neighboring double wells during the irradiation time $t_{\text{PA}} = 0.5$ ms of the PA laser. The quantity $2t_{\text{PA}}t/\hbar$ is a measure of the number of inter-dimer hopping events during the PA laser irradiation time, which is plotted as the red solid curve in Fig. 5.11(a), and the black dashed line represents the value of 1. It can be qualitatively understood that this suppression is due to the combined effect of on-site two-body losses and holes created by tunneling between double wells. The previous work [84] has also pointed out that numerically calculated spin correlations between nearest-neighbor sites of a 1D uniform lattice are smaller than those of an isolated double-well lattice. Special emphasis is given to the result for the 1D uniform lattice ($s_{\text{long}}^{(z)} = 0$), where $A = -0.010(6)$ is small but definitely nonzero and negative. In Fig. 5.11(b), we show the STO signal for another 1D uniform lattice, where $A = -0.023(5)$ is negative as well. These results clearly indicate that in the 1D uniform lattice, the magnetic

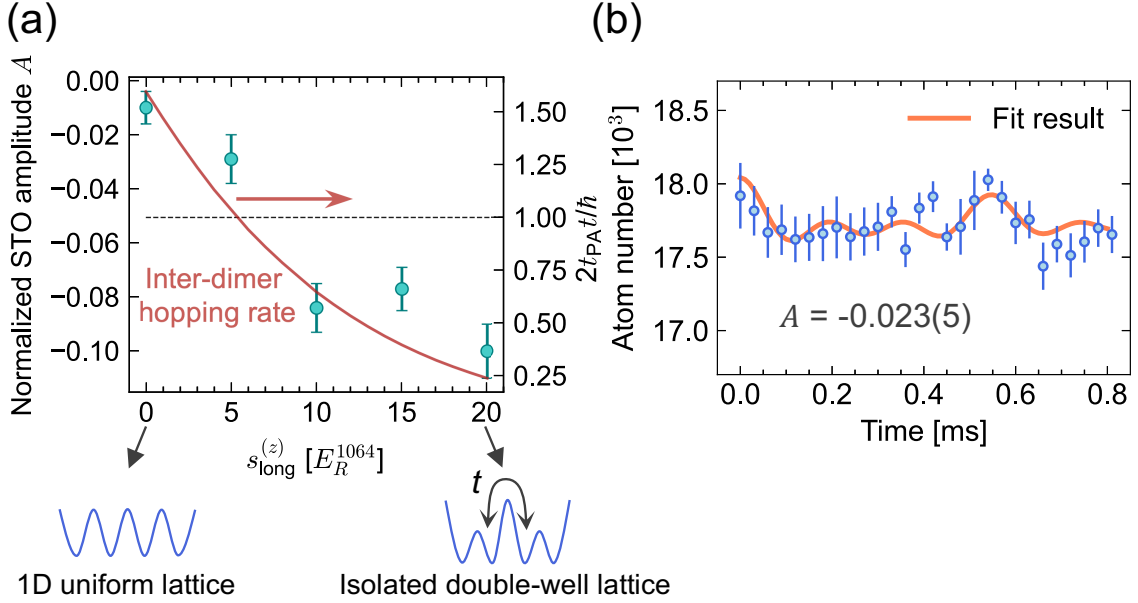


Figure 5.11: (a) Normalized STO amplitude A in a crossover from an isolated double-well lattice of $s_L = [100, 80, (20.8, 20)]$ to a 1D uniform lattice of $s_L = [100, 80, (20.8, 0)]$. Here, the dependency of A on the long lattice depth is shown. We note that the number of scans in STO measurement at $s_{\text{long}}^{(z)} = 0 E_R^{1064}$ is seventeen, otherwise three. The red solid curve shows the quantity $2t_{\text{PA}} t/\hbar$, which is a measure of the number of inter-dimer hopping events during the PA laser irradiation time, and the black dashed line represents the value of 1. Here, the factor 2 corresponds to tunnelings to double wells on both sides. (b) Measured STO signal in a 1D uniform lattice of $s_L = [100, 80, (8, 0)]$. The orange solid curve shows the fit result. Error bars denote the standard error of twelve scans. Figure adapted from Ref. [194].

correlation also reverses, and the ferromagnetic correlation emerges. For all lattice configurations dealt with in this measurement, the steady state is expected to be the Dicke state. However, steady states are considered unachieved in this measurement as the right axis in Fig. 5.11(a) shows that the irradiation time of the PA laser is comparable with the inter-dimer hopping time, which is the consequence of the restriction of the irradiation time of the PA laser for the reasons mentioned above. So far, in a dissipative 1D uniform lattice, the formation of the Dicke state, which has a fully symmetric spin wave function and shows a ferromagnetic correlation, has only been indirectly suggested based on the atom loss dynamics [88]. The observed ferromagnetic correlation in this work provides a signature of the formation of Dicke type of correlations in the long-time limit.

5.7 Summary and outlook

In this work, we implement a driven-dissipative Fermi-Hubbard system with on-site two-body losses, utilizing a PA technique. We systematically measure the dynamics of the nearest-

neighbor spin correlation in an isolated double-well optical lattice, as well as a crossover from an isolated double-well lattice to a one-dimensional uniform lattice. In a wide range of lattice configurations over an isolated double-well lattice, we observe a ferromagnetic spin correlation, which is consistent with a Dicke type of correlation expected in the long-time limit. This work demonstrates the control of quantum magnetism in open quantum systems with dissipation. In higher dimensions (2D and 3D), the spin-charge separation does not occur. Thus, the behavior of the long-range magnetic correlation in a dissipative 2D or 3D system is an interesting problem as a future outlook.

OBSERVATION OF SLOW RELAXATION DUE TO HILBERT SPACE FRAGMENTATION IN STRONGLY INTERACTING BOSE-HUBBARD CHAINS

In this chapter, we report an experimental study of the nonequilibrium dynamics following the sudden quench in the one-dimensional Bose-Hubbard system with neither disorder nor tilt potential. Especially, we successfully observe a slowing-down of the relaxation in a strongly interacting regime starting from a charge-density wave of doublons, and find that the numbers of singlons and doublons are conserved during the dynamics, indicating HSF as a mechanism of the observed slow relaxation. We first describe the sample preparation, sudden quench of the lattice depth, and measurement of the atom number imbalance in Sec. 6.1. Then, in Sec. 6.2, we show the experimental results of the imbalance measurement and doublon- and singlon-fraction measurement in the quench dynamics, along with the comparison between experiments and numerical calculations. Also, we show the experimental results for the effect of singlons on the imbalance dynamics. Theoretical calculations were carried out by Dr. Shimpei Goto, Dr. Masaya Kunimi, and Dr. Ippei Danshita.

6.1 Experimental setup

6.1.1 Initial state preparation

A BEC of ^{174}Yb is prepared by evaporative cooling in a crossed dipole trap operating at a wavelength of 532 nm, where the total atom number is about 1.3×10^4 . The frequencies of the dipole trap are given by $\omega_{x+y}/(2\pi) = 27$ Hz, $\omega_{x-y}/(2\pi) = 95$ Hz, and $\omega_z/(2\pi) = 109$ Hz, respectively. Note that the axes in the xy plane of the dipole trap are directed at 45

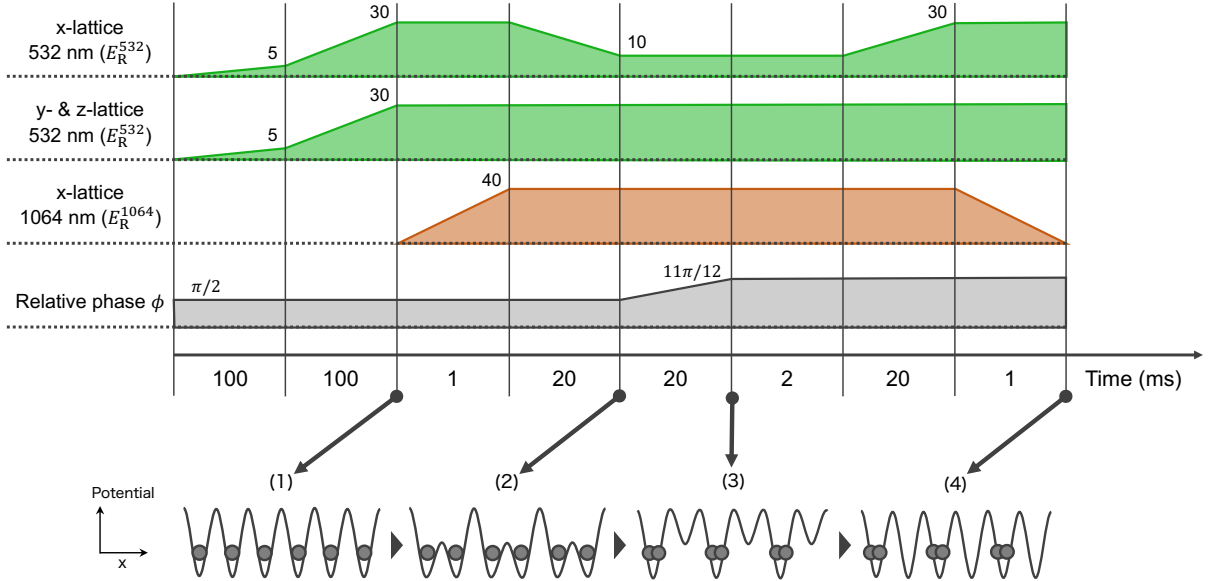


Figure 6.1: Schematic illustration and timing diagram of the preparation procedure for $\hat{\rho}_{\text{CDW(d)}}(0)$ state in 1D chains.

degrees to those of the optical lattice potential. Then, we load it into a 3D cubic optical lattice with a deep potential depth of $s_L = [(s_{\text{short}}^{(x)}, s_{\text{long}}^{(x)}), s_{\text{short}}^{(y)}, s_{\text{short}}^{(z)}] = [(30, 0), 30, 30]$ in 200 ms, where $s_{\text{short}}^{(x,y,z)}$ and $s_{\text{long}}^{(x)}$ are the potential depth of the short and the long lattice normalized by the recoil energy $E_R = \hbar^2 k_L^2 / (2m)$ ($k_L = 2\pi/\lambda$) for each wavelength λ , respectively. The optical lattice depth is calibrated by observing the diffraction caused by a pulsed optical lattice [178]. Here, a Mott insulating state of unit filling is formed (stage (1) in Fig. 6.1). The optical-lattice potential at $s_L = [(30, 0), 30, 30]$ also acts as a parabolic trapping potential, whose frequencies are given by $\tilde{\omega}_x/(2\pi) = 66$ Hz, $\tilde{\omega}_y/(2\pi) = 71$ Hz, and $\tilde{\omega}_z/(2\pi) = 58$ Hz. Here, the preparation of the initial state of period-two CDW of doublons, i.e., $|\psi(0)\rangle_{\text{CDW(d)}} = |\cdots 2020 \cdots\rangle$ state in 1D chains proceeds with the optical superlattice in the direction of 1D chains consisting of short ($\lambda_{\text{short}} = 532$ nm) and long ($\lambda_{\text{long}} = 1064$ nm) lattices, as follows. Note that for representing the many-body state of a 1D chain with M sites, here we use the Fock basis,

$$|n_1 n_2 \cdots n_M\rangle \equiv \bigotimes_{i=1}^M |n_i\rangle_i, \quad (6.1)$$

where $|n_i\rangle_i$ denotes the local Fock state at a site i with an atom number n_i .

(2) Ramp up the long lattice and trap the atoms in an optical superlattice in a double-well condition along the 1D chains, where the relative phase between the short and the long lattice is $\pi/2$, and ramp down the short lattice to form the relatively shallow double-well lattice of $s_L = [(10, 40), 30, 30]$ in about 20 ms.

(3) Sweep the relative phase of the short and the long lattice from $\pi/2$ to near π , or staggered condition, in 20 ms, where atoms in the right side of a double-well are transferred to the left side (stage (3) in Fig. 6.1).

(4) Ramp up the short lattice in 20 ms and then ramp down the long lattice in 1 ms to the potential depth of $s_L = [(30, 0), 30, 30]$, where $\hat{\rho}_{\text{CDW(d)}}(0)$ state is to be prepared. Here, the central 1D chains of the atoms have a length of about 25.

As mentioned in the main text, 25-30% of total atoms in the prepared state are singlons. This is confirmed with the irradiation of a PA laser, where we use a PA line about 3.7 GHz below the $^1S_0 \leftrightarrow ^3P_1$ resonance [204]. Note that, we estimate the singlon fraction in the initial $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state based on the atom density distribution at the Mott insulating state in $s_L = [(30, 0), 30, 30]$ in the atomic limit (Fig. 6.2(b) (left)). In the calculation, we first obtain the temperature in the optical lattice T (the temperature of the Mott insulating state) and the chemical potential μ by solving the following simultaneous nonlinear equations:

$$\begin{cases} N_{\text{exp}} = N(T, \mu) = -\frac{\partial \Omega(T, \mu)}{\partial \mu}, \\ S_{\text{exp}} = S(T, \mu) = -\frac{\partial \Omega(T, \mu)}{\partial T}. \end{cases} \quad (6.2)$$

$$\quad (6.3)$$

Here, $\Omega(T, \mu)$ is the grand potential given as follows:

$$\Omega(T, \mu) = -\beta \sum_i \ln(z_i), \quad (6.4)$$

$$z_i = \sum_{k=0}^{m_t} \exp \left[-\beta \left(\frac{U}{2} k(k-1) + \left(\mu - \frac{1}{2} m \omega^2 d^2 r_i^2 \right) k \right) \right], \quad (6.5)$$

where i is the lattice site index; $\beta = (k_B T)^{-1}$; U is the on-site interaction strength; ω is the geometric mean of the trap frequency; d is the lattice constant; and m_t is the truncation filling. Also, N_{exp} and S_{exp} are the total atom number and total entropy of the Mott insulating state, respectively. In particular, the total entropy S_{exp} is estimated as the half of the entropy measured after the ‘round-trip’ process, where we first ramp up the lattice to $s_L = [(30, 0), 30, 30]$ and then completely ramp down the lattice (Fig. 6.2(a)), and we obtain $S/N_{\text{exp}} k_B = 0.23$. Note that in an actual calculation, we solve Eqs. (6.2) and (6.3) under the continuous approximation ($\sum_i f(r_i) = (1/d^3) \int_0^\infty dr 4\pi r^2 f(r/d)$) as follows:

$$\begin{cases} N_{\text{exp}} \sim \frac{1}{d^3} \int_0^\infty dr 4\pi r^2 \left[\frac{1}{z(r)} \sum_{k=0}^{m_t} k \exp \left\{ -\beta \left(\frac{U}{2} k(k-1) + \left(\mu - \frac{1}{2} m \omega^2 r^2 \right) k \right) \right\} \right], \\ S_{\text{exp}} \sim \frac{k_B N_{\text{exp}}}{d^3} \int_0^\infty dr 4\pi r^2 \left[\ln(z(r)) \right. \\ \quad \left. + \frac{\beta}{z(r)} \left\{ \sum_{k=0}^{m_t} \left(\frac{U}{2} k(k-1) + \left(\mu - \frac{1}{2} m \omega^2 r^2 \right) k \right) \exp \left(-\beta \left(\frac{U}{2} k(k-1) + \left(\mu - \frac{1}{2} m \omega^2 r^2 \right) k \right) \right) \right\} \right]. \end{cases} \quad (6.6)$$

Under the condition of $\omega = 2\pi \times 118$ Hz, $U/h = 4.74$ kHz, $N_{\text{exp}} = 1.3 \times 10^4$, and $S_{\text{exp}}/N_{\text{exp}} k_B = 0.23$, we obtain $T = 4.1$ nK and $\beta\mu = 21$. Using these values, we calculate the singlon fraction

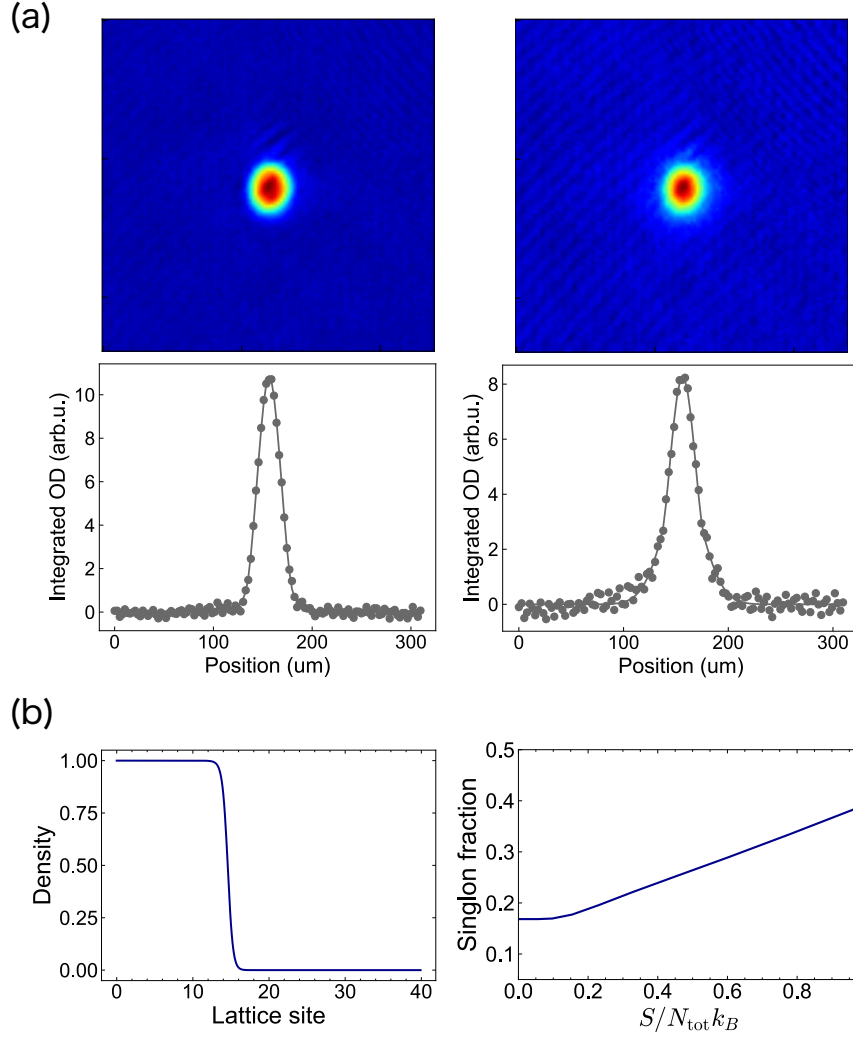


Figure 6.2: Estimation of the singlon fraction in the initial $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state. (a) Absorption image and its vertically integrated OD for before (left) and after (right) ‘round-trip’ process, taken after 14 ms time of flight. Both images are the average of five data. Solid curves in the lower left and lower right are the results of the bimodal fit. (b) Calculated atom density for the temperature of 4.1 nK in the Mott insulator state, which corresponds to the entropy per particle $S/N_{\text{tot}}k_B$ of 0.23 (left), and singlon fraction as a function of the entropy per particle (right).

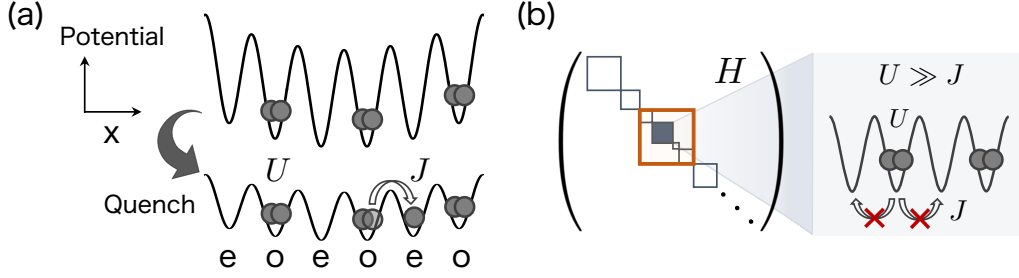


Figure 6.3: (a) Schematic of the 1D Bose-Hubbard model with a tunneling amplitude J , an on-site interaction strength U , and a parabolic trap with no potential tilt. Here, the ideal initial state of a period-two charge-density wave of doublons, namely, $|\psi(0)\rangle_{\text{CDW(d)}} = |\cdots 2020 \cdots\rangle$ is shown. (b) Schematic illustration of HSE. The orange square shows a subspace characterized by the particle number. This subspace is further fragmented into an exponentially large number of subsectors (Krylov subsectors) under some kinetic constraints, where the breakup of doublons into singlons due to tunneling is suppressed for $U \gg J$ due to the energy mismatch in our case.

as $1 - N_{\text{doublon}}/N_{\text{tot}} = 1 - 2 \sum_i 4\pi(2i)^2 \cdot p_{2i} \cdot p_{2i+1}$, where p_i is the atom density (site occupancy probability of the singlon) at a site i , and is given as follows:

$$p_i = \frac{1}{z_i} \sum_{k=0}^{m_i} k \exp \left\{ -\beta \left(\frac{U}{2} k(k-1) + \left(\mu - \frac{1}{2} m \omega^2 d^2 r_i^2 \right) k \right) \right\}. \quad (6.8)$$

As a result, we obtain the singlon fraction of 20% for the temperature of 4.1 nK in the Mott insulator state, which corresponds to the entropy per particle $S/N_{\text{tot}} k_B$ of 0.23, where k_B is the Boltzmann constant (Fig. 6.2(b) (right)). Here, the slight deviation from the measured singlon fraction of 25-30% may be due to the presence of low-density regions at the trap edges and the nonadiabaticity in the loading process after the preparation of the Mott insulating state.

6.1.2 Sudden quench of the lattice depth

After the initial state preparation, we ramp up the potential depth in the directions perpendicular to the 1D chains from $s_L = [(30, 0), 30, 30]$ to $[(30, 0), 40, 40]$ in 1 ms, and then perform a sudden quench to $s_L = [(s_{\text{short}}^{(x)}, 0), 40, 40]$ in 0.1 ms to initiate the dynamics along the 1D chains (see Fig. 6.3(a)). Note that in the measurement of dependency of quench dynamics on U/J , described in Sec. 6.2.2, the sweep time for quench is fixed to the above value independent of the potential depth along the 1D chains after the quench. We also note that we numerically confirm that even when the change in the potential depth is maximal ($U/J = 12$ case), the occupation probability of the ground state of the optical lattice potential after the quench exceeds 0.99 at least for singly occupied sites. The dynamics

during the hold time in the 1D chains is described by the 1D Bose-Hubbard model, and the Hamiltonian is given by

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_{i=1}^M \hat{n}_i (\hat{n}_i - 1) + \sum_{i=1}^M V_i \hat{n}_i, \quad (6.9)$$

where $\hat{a}_i$ ($\hat{a}_i^\dagger$) is the annihilation (creation) operator of a boson at a site i ; J is the tunneling amplitude between nearest-neighbor sites $\langle i, j \rangle$; $\hat{n}_i \equiv \hat{a}_i^\dagger \hat{a}_i$ is the number operator at a site i ; U is the on-site interaction strength; $V_i \equiv \Omega[i - (M+1)/2]^2$ is the parabolic potential; and Ω is the strength of the parabolic potential [138]. Here, we note that there is no tilt potential in Eq. (6.9), different from previous experimental studies of nonergodic dynamics due to the HSF [129, 130, 134] and the many-body scarring [120]. Note that the relative strength of the parabolic potential Ω to the tunneling amplitude J depends on the lattice depth (See Tables 6.1 and 6.2), and Ω is small compared with hopping J of the singlon but not with that of the doublon.

6.1.3 Atom number imbalance measurement

In order to detect the atom distribution after the quench, we freeze the dynamics by rapidly ramping up the potential depth along the 1D chains in 0.1 ms to $s_{\text{short}}^{(x)} = 30$. In this work, we focus on two physical quantities that characterize the atom distribution: atom-number imbalance $I(t)$ between the odd and even sites, and doublon- and singlon-resolved atom-number fraction (n_D, n_S). The imbalance $I(t)$ is defined as

$$I(t) \equiv \frac{N_{\text{odd}}(t) - N_{\text{even}}(t)}{N_{\text{odd}}(t) + N_{\text{even}}(t)}, \quad (6.10)$$

which becomes zero for thermalized states, where $N_{\text{odd}}(t)$ and $N_{\text{even}}(t)$ are the atom numbers in the odd and even sites, respectively. The measurement of the imbalance is performed by a site-mapping technique; i.e., mapping of the even and odd sites to the 1st and 3rd bands, respectively, followed by band mapping [205, 206, 129, 130], as follows (see Fig. 6.4: We ramp up the long lattice to $s_{\text{long}}^{(x)} = 40$ in 1 ms, and then completely ramp down the short lattice in 1 ms. Here, we map the particle position, i.e., the odd and even sites, to the 1st and the 3rd band of the potential of the long lattice, respectively [206]. Then, the band-mapping is performed in 0.6 ms, and the imbalance I is derived from the obtained band-mapping image. Note that in our analysis, we count the atom numbers in the "1st BZ + half of the 2nd BZ on the closer side to the 1st BZ" and "3rd BZ + half of the 2nd BZ on the closer side to the 3rd BZ" as N_{odd} and N_{even} , respectively, taking into account the possible imperfection of our band-mapping process, although the 2nd BZ population is small. We also note that we observe a slight deviation of imbalance from zero ($I_{\text{offset}} = 0.082(3)$) when we start the quench dynamics from $|\cdots 1111 \cdots\rangle$ state as a reference state which should show zero imbalance. This might be due to the imperfection of the particle position mapping or the band-mapping. In our analysis, we subtract this offset from the obtained imbalance I .

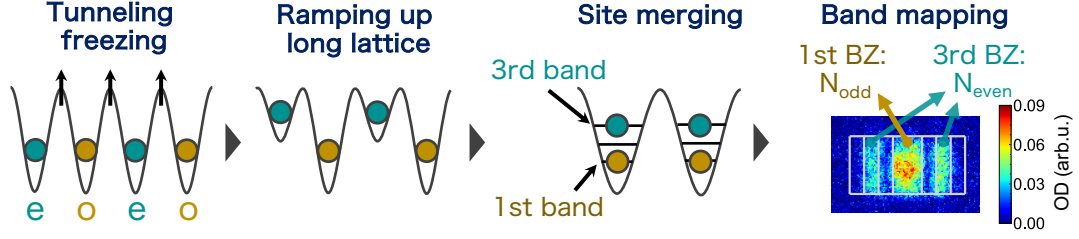


Figure 6.4: Schematic illustration of the sequence for a site-mapping technique to measure the atom number imbalance. In this illustration, atoms in the odd (even) sites are mapped to the 1st (3rd) Brillouin zone (BZ).

Note that, as we mention in the state preparation, the prepared state is not a pure state $|\psi(0)\rangle_{\text{CDW(d)}}$, but a mixed state $\hat{\rho}_{\text{CDW(d,s)}}(0)$, which involves singlons with 25-30% of total atoms. By exploiting the PA resonance, which selectively excites and thus removes the doublons, we achieve measurements of the imbalance in a singlon- and doublon-resolved manner [206, 130]. Specifically, we measure the imbalance with and without the PA laser irradiation just after the freezing of the dynamics and before the site-mapping, where the imbalance of singlons ($I_{\text{w/PA}} = I_{\text{S}}$) and that of both doublons and singlons ($I_{\text{w/oPA}}$) are obtained, respectively. Then, we obtain the imbalance of doublons (I_{D}) from the former two measured values as follows:

$$I_{\text{D}} = \frac{I_{\text{w/oPA}} \cdot N_{\text{w/oPA}} - I_{\text{w/PA}} \cdot N_{\text{w/PA}}}{N_{\text{w/oPA}} - N_{\text{w/PA}}}, \quad (6.11)$$

where $N_{\text{w/PA}}$ ($N_{\text{w/oPA}}$) is the atom number measured with (without) PA laser irradiation. Note that I_{D} is calculated with calibrated values of $I_{\text{w/PA}}$ and $I_{\text{w/oPA}}$ considering the offset of the imbalance, mentioned above. The doublon- and singlon-resolved atom number fraction, n_{D} and n_{S} , are obtained with the atom numbers measured with and without the PA laser irradiation, $N_{\text{w/PA}}$ and $N_{\text{w/oPA}}$, as follows:

$$n_{\text{S}} = N_{\text{w/PA}} / N_{\text{w/oPA}}, \quad (6.12)$$

$$n_{\text{D}} = (N_{\text{w/oPA}} - N_{\text{w/PA}}) / N_{\text{w/oPA}}. \quad (6.13)$$

Note that these atom number fractions are important to characterize the nonequilibrium dynamics in the sense that they are emergent conserved quantities in the strongly interacting regime of the Bose-Hubbard chain, leading to the HSF [138].

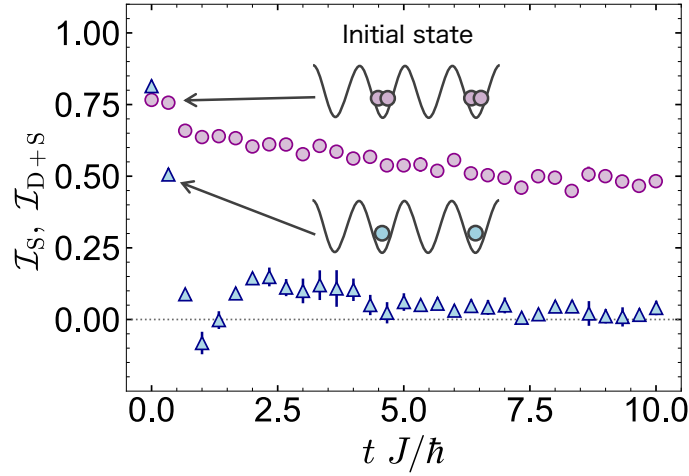


Figure 6.5: Comparison of quench dynamics at $U/J = 52$ starting from $\hat{\rho}_{\text{CDW(d,s)}}(0)$ (purple circle) and $\hat{\rho}_{\text{CDW(s)}}(0)$ (blue triangle). The horizontal axis represents the holding time after the quench normalized by the tunneling time of $\hbar/J = 2.6$ ms along the direction of the 1D chains. Error bars in I_{D+S} and I_S show the standard deviation of three and five independent scans, respectively.

6.2 Experimental results

6.2.1 Typical quench dynamics: slow imbalance relaxation, and doublon- and singlon-fraction conservation

We first show the comparison of the thermalization behaviors obtained at $U/J = 67$ starting from the $\hat{\rho}_{\text{CDW(d,s)}}(0)$ and $\hat{\rho}_{\text{CDW(s)}}(0)$ states in Fig. 6.5 (see Sec. 6.2.4 for the details of the quench dynamics starting from the $\hat{\rho}_{\text{CDW(s)}}(0)$ state). Here, $\hat{\rho}_{\text{CDW(s)}}(0)$ denotes an initial mixed state that is in reality created when we try to ideally prepare

$$|\psi(0)\rangle_{\text{CDW(s)}} = |\cdots 1010 \cdots\rangle. \quad (6.14)$$

In Fig. 6.5, the imbalance I shows slow relaxation and remains far from zero at least up to ten times of the tunneling time along the 1D chains when the initial state is $\hat{\rho}_{\text{CDW(d,s)}}(0)$, while the imbalance shows rapid relaxation and an oscillating behavior across zero when the initial state is $\hat{\rho}_{\text{CDW(s)}}(0)$. These different relaxation behaviors are theoretically discussed in Ref. [138], where the nonergodic dynamics is expected when the initial state is $|\psi(0)\rangle_{\text{CDW(d)}} = |\cdots 2020 \cdots\rangle$. Note that although the relaxation behavior in the 1D Bose-Hubbard system when the initial state is approximately $|\cdots 1010 \cdots\rangle$ has already been reported in Ref. [207], we revisit this situation to show a clear difference in the quench dynamics depending on the initial states.

In the following, for the quantitative study, we focus on the quench dynamics starting from the $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state. In Fig. 6.6(a), we show the typical quench dynamics of the im-

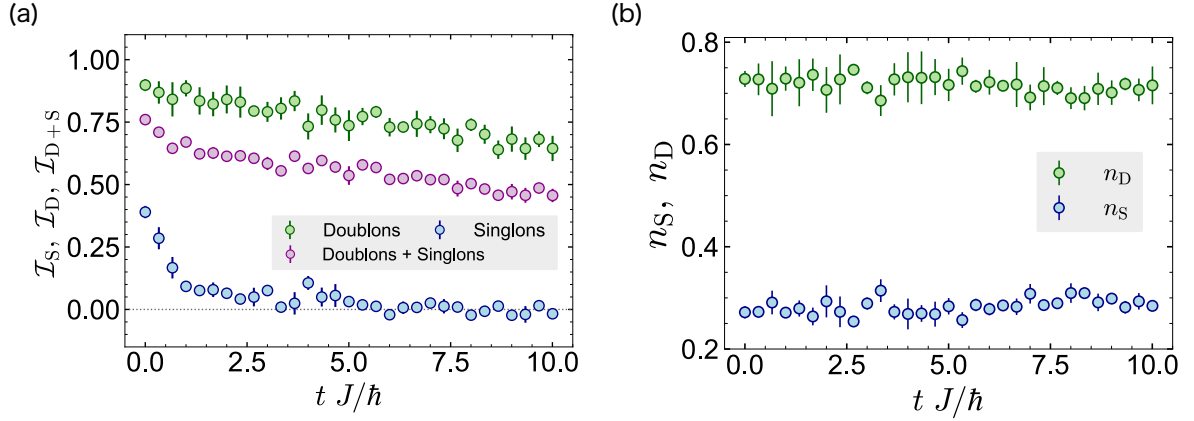


Figure 6.6: (a) Typical dynamics of imbalances of ‘Doublons + Singlons’ (purple), ‘Singlons’ (blue) obtained by the PA irradiation, and ‘Doublons’ (green) obtained from the former two. (b) Typical dynamics of atom number fractions of doublons (n_D , green) and singlons (n_S , blue). In (a) and (b), all data are obtained at $U/J = 67$, and the horizontal axis represents the holding time normalized by the tunneling time of $\hbar/J = 2.1$ ms along the direction of the 1D chains. In (a), error bars in ‘Doublons + Singlons’ and ‘Singlons’ show the standard deviation of three independent scans, and that in ‘Doublons’ show the standard deviation, which is calculated by the error propagation formula with the standard deviations of $I_{W/PA}$, $I_{W/O PA}$, $N_{W/PA}$ and $N_{W/O PA}$. In (b), error bars show the standard deviation, which is calculated by the error propagation formula with the standard deviations of $N_{W/PA}$ and $N_{W/O PA}$.

balances of both doublons and singlons (‘Doublons+Singlons’, I_{D+S}), singlons (‘Singlons’, I_S), and doublons (‘Doublons’, I_D) obtained from the former two by Eq. (6.11), where $U/J = 67$. Here, the imbalances of doublons and singlons show slow and rapid relaxation, respectively. Note that tunneling time along the direction perpendicular to the 1D chains is $\hbar/(4J_\perp) = 92$ ms, about 3.5 times longer than the maximum measurement time. In addition to the successful observation of the slow relaxation behavior for doublons, we observe that both of the atom number fractions of doublons (n_D) and singlons (n_S) are almost conserved, as shown in Fig. 6.6(b). This reveals that the atom numbers of both doublons and singlons serve as approximate conserved quantities, which is a key finding in the sense that this strongly supports the occurrence of HSF in our system, where the dissociation of doublons due to single particle tunnelings is suppressed for $U \gg J$ due to the energy mismatch (see Fig. 6.3(b)).

6.2.2 Dependency of quench dynamics on U/J

In order to elucidate the role of interatomic interaction as well as the interplay with the parabolic potential in the nonequilibrium dynamics, we investigate the dependency of the

$s (E_R)$	J/h (Hz)	U/J	$2J^2/U$ (Hz)	Ω/J
5	266	12	44.3	0.037
8	125	30	8.33	0.079
10	77.7	52	2.99	0.13
11	61.9	67	1.85	0.16
12	49.6	86	1.15	0.20
14	32.4	138	0.470	0.31
15	26.4	173	0.305	0.38

Table 6.1: Bose-Hubbard parameters for the systematic measurement shown in Fig. 6.7.

quench dynamics on the interaction strength U/J and the parabolic trap strength Ω/J by changing the potential depth along the 1D chains after the quench, shown in Fig. 6.7(a)-(c). Bose-Hubbard parameters for this systematic measurement are listed in Table 6.1. Here, the tunneling amplitude J , U/J , and $2J^2/U$ are obtained from the first principle calculation for an optical lattice potential. The harmonic potential strength $\Omega = m\omega^2 d^2/2$ is obtained by the trap frequency along the axial direction of a 1D chain ($\omega = 2\pi \times 128$ Hz), the mass m of ^{174}Yb atoms, and the lattice constant $d = 266$ nm. In Fig. 6.7(a) and (b), we observe an overall tendency of slower relaxation of the imbalance of doublons for larger U/J , while the imbalance of singlons shows fast relaxation roughly independent of U/J . At the same time, in Fig. 6.7(c), we observe that the atom number fractions of both doublons and singlons are almost conserved regardless of the value of U/J (see also Fig. 6.8). These results can be understood intuitively as follows: Recall that the dissociation of a doublon into two singlons is approximately forbidden, as assured by the conservation of the fractions. In the cases of relatively small U/J , not only singlons can tunnel to adjacent vacant sites with the tunneling rate of J , but also doublons via the process of the second-order perturbation with the effective tunneling rate of $J_{\text{eff}} = 2J^2/U$, as depicted in Fig. 6.9(b), on the one hand. In fact, the time constant of the correlated tunneling, $\hbar/(2J_{\text{eff}})$ is $3\hbar/J$ for the smallest U/J case ($U/J = 12$), where the factor of 2 in front of J_{eff} means the number of nearest-neighboring sites along the chain direction. In the cases of relatively large U/J , on the other hand, the rate of the effective hopping of the doublon becomes quite small, corresponding to about 1/5-time hopping event during the maximum holding time, for largest U/J case ($U/J = 173$), and thus only singlon tunneling is allowed, as in Fig. 6.9(a). Note that the effect of the parabolic trap also contributes to the suppression of the doublon tunneling, while such an effect is considerably weaker for singlons.

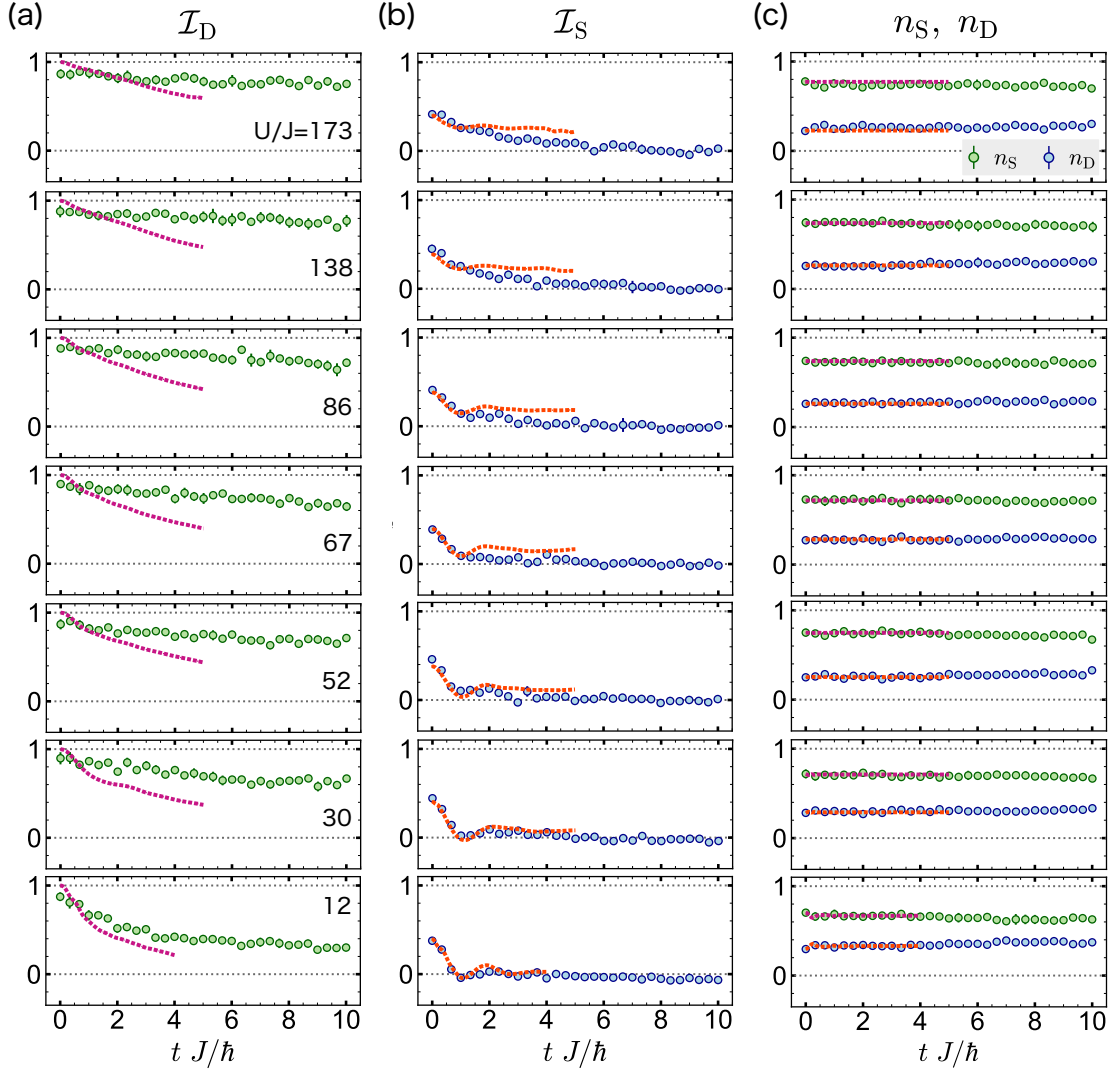


Figure 6.7: Dependence of quench dynamics on U/J . (a),(b) Imbalance dynamics of (a) doublons (I_D), (b) singlons (I_S), and (c) atom number fractions of doublons (n_D , green) and singlons (n_S , blue) on U/J . Error bars in (a)-(c) representing the standard deviation are mostly smaller than symbols. In (a)-(c), dotted curves show the calculated values. Error bars of calculated values representing the statistical error are smaller than the dots of the curves.

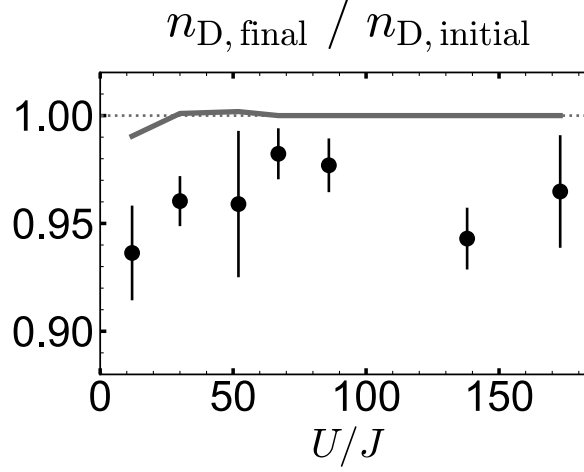


Figure 6.8: Change of the doublon fraction during the hold time. Here, the ratio of the averaged doublon fraction in $tJ/\hbar = 9-10$ ($n_{D,\text{final}}$) to that in $tJ/\hbar = 0-1$ ($n_{D,\text{initial}}$) is plotted. Error bars show the standard deviation, which is calculated by the error propagation formula with the standard deviation of the averaged doublon fractions $n_{D,\text{initial}}$ and $n_{D,\text{final}}$. The solid curve shows the ratio of the calculated averaged doublon fraction in $tJ/\hbar = 4-5$ ($tJ/\hbar = 3-4$ only in the case of $U/J = 12$) ($n_{D,\text{final}}$) to that in $tJ/\hbar = 0-1$ ($n_{D,\text{initial}}$).

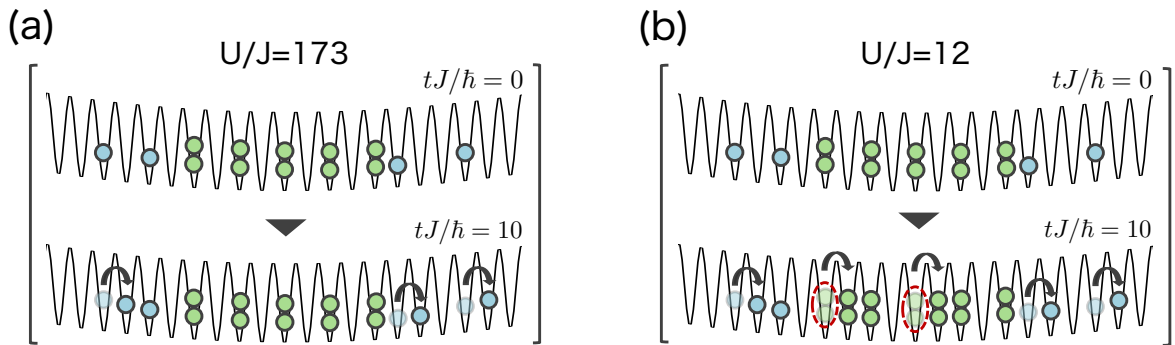


Figure 6.9: Schematic illustration of tunneling dynamics of doublons and singlons in a lattice for relatively (a) small and (b) large U/J cases.

6.2.3 Comparison between experiments and numerical calculations

In order to provide a reference to be compared with the experimental results, we compute the real-time dynamics of the 1D Bose-Hubbard model of Eq. (6.9) by using the time-evolving block decimation (TEBD) method [208], which is based on matrix-product state (MPS) representation of a quantum many-body state [209]. We set the maximal bond dimensions of MPS to be 2000 such that the time duration accessible with the numerical calculations is as short as or even shorter than the half of that in the experiments. In Fig. 6.7, we show the direct comparison of measured and calculated values of (a) doublon- and (b) singlon-resolved imbalance (I_D and I_S) and (c) doublon and singlon fractions (n_D and n_S) for several values of U/J . Here, the calculation reflects the realistic situation in the experiment. We find that the behaviors of both imbalance and atom number fraction are mostly reproduced by the theoretical calculations, confirming that the dynamics of our experimental system are indeed well-described by the 1D Bose-Hubbard model.

6.2.4 Quench dynamics starting from $\hat{\rho}_{\text{CDW(s)}}(0)$ state

In the measurement of the quench dynamics from the $\hat{\rho}_{\text{CDW(s)}}(0)$ state shown in Fig. 6.5, we use the following parameters in the state preparation, lattice quench, and imbalance measurement. Recall that $\hat{\rho}_{\text{CDW(s)}}(0)$ is a mixed state created in reality when we try to prepare the ideal $|\psi(0)\rangle_{\text{CDW(s)}} = |\cdots 1010 \cdots\rangle$ state.

First, we load ^{174}Yb BEC into a 3D cubic optical lattice with a deep potential depth of $s_L = [(0, 40), 25, 25]$ in 300 ms, where the total atom number is about 4.5×10^3 . Here, a Mott insulating state of unit-filling is formed (stage (1) in Fig. 6.10). The optical-lattice potential at $s_L = [(0, 40), 25, 25]$ also acts as a parabolic trapping potential, whose frequencies are given by $\tilde{\omega}_x/(2\pi) = 37$ Hz, $\tilde{\omega}_y/(2\pi) = 65$ Hz, and $\tilde{\omega}_z/(2\pi) = 53$ Hz. Then, we ramp up the short lattice in 1 ms and trap the atoms in an optical superlattice in a staggered condition along the 1D chains, followed by ramping down of the long lattice in 1 ms, where the $\hat{\rho}_{\text{CDW(s)}}(0)$ state is prepared in the potential depth of $s_L = [(25, 0), 25, 25]$ (stage (3) in Fig. 6.10). Note that we confirm that the fraction of the doublons involved in this initial state $|\psi(0)\rangle_{\text{CDW(s)}}$ is smaller than our detection limit of about 5% with the PA method. For this state, we perform a sudden quench to $s_L = [(s_{\text{short}}^{(x)}, 0), 25, 25]$ in 0.15 ms, where the tunneling time along the direction perpendicular to the 1D chains is 38 ms. In order to detect the imbalance after the dynamics, we freeze the atom distribution by rapidly ramping up the potential depth along the 1D chains in 0.1 ms to $s_{\text{short}}^{(x)} = 25$, and then we ramp up the long lattice to $s_{\text{long}}^{(x)} = 40$ in 1 ms, and finally completely ramp down the short lattice in 1 ms, followed by the band-mapping in 0.6 ms. Note that in the imbalance measurement in the above parameters, we observe a slight deviation of imbalance from zero ($I'_{\text{offset}} = 0.117(3)$) when we start the quench dynamics from $|\cdots 1111 \cdots\rangle$ state, which is subtracted from the obtained imbalance.

In Fig. 6.11, we show the results of the quench dynamics from $\hat{\rho}_{\text{CDW(s)}}(0)$ state, where the dependency of imbalance dynamics on U/J is systematically measured. Here, the cal-

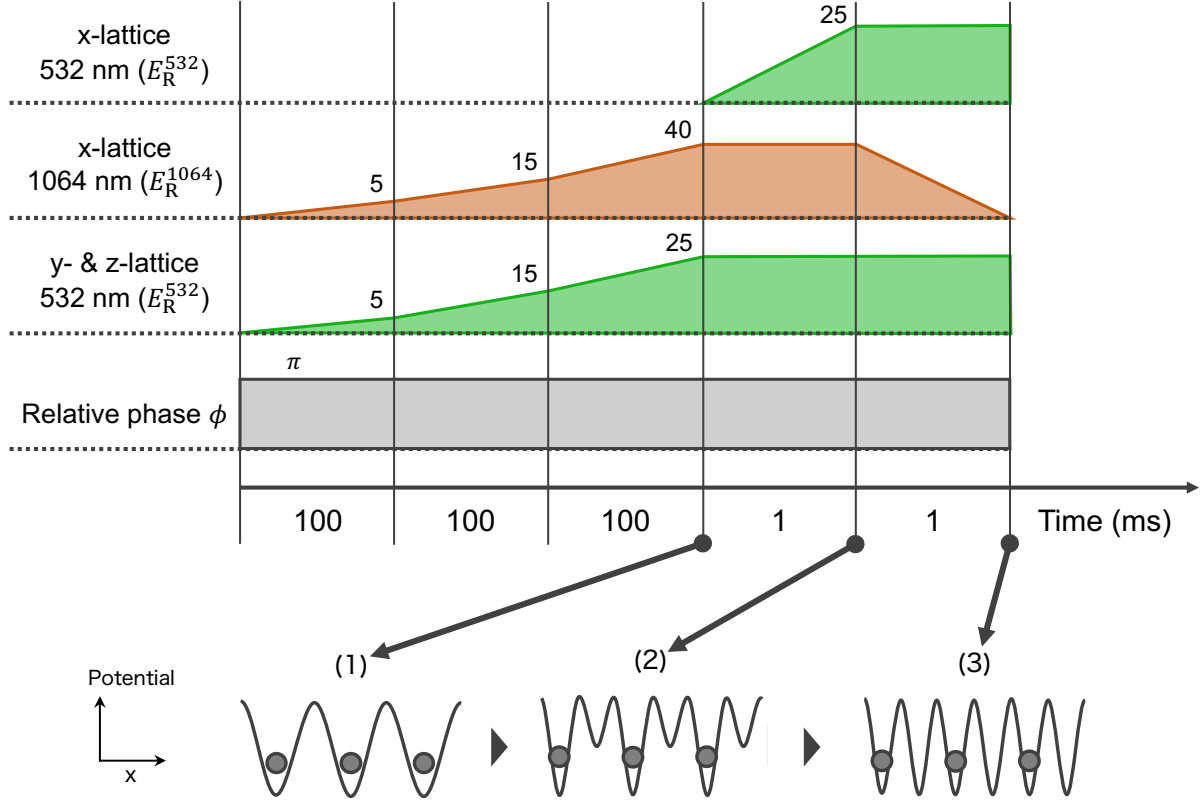


Figure 6.10: Schematic illustration and timing diagram of the preparation procedure for $\hat{\rho}_{CDW(s)}(0)$ state in 1D chains.

culation reflects the realistic situation in the experiment. Bose-Hubbard parameters for this systematic measurement are listed in Table 6.2, where the trap frequency along the axial direction of a 1D chain is $\omega = 2\pi \times 109$ Hz in this case. We find that the measured imbalance values are mostly reproduced by the theoretical calculations.

6.2.5 Competition among doublon-doublon interactions, doublon-singlon interactions, and a parabolic trap in the imbalance dynamics

While we see the agreement between the experimental data and theoretical calculations, here we discuss how much extent the experimental results can be understood in an intuitive manner and clarify the novelty beyond simple interpretations. Specifically, we first see whether we can understand in a unified manner the dynamics of the singlons and doublons by regarding both of them as simple non-interacting hardcore bosons with the corresponding effective tunneling amplitude $J_{\text{eff}} = J$ for the singlons and $J_{\text{eff}} = 2J^2/U$ for the doublons placed in a parabolic trap with the trap strength Ω , thus characterized only by

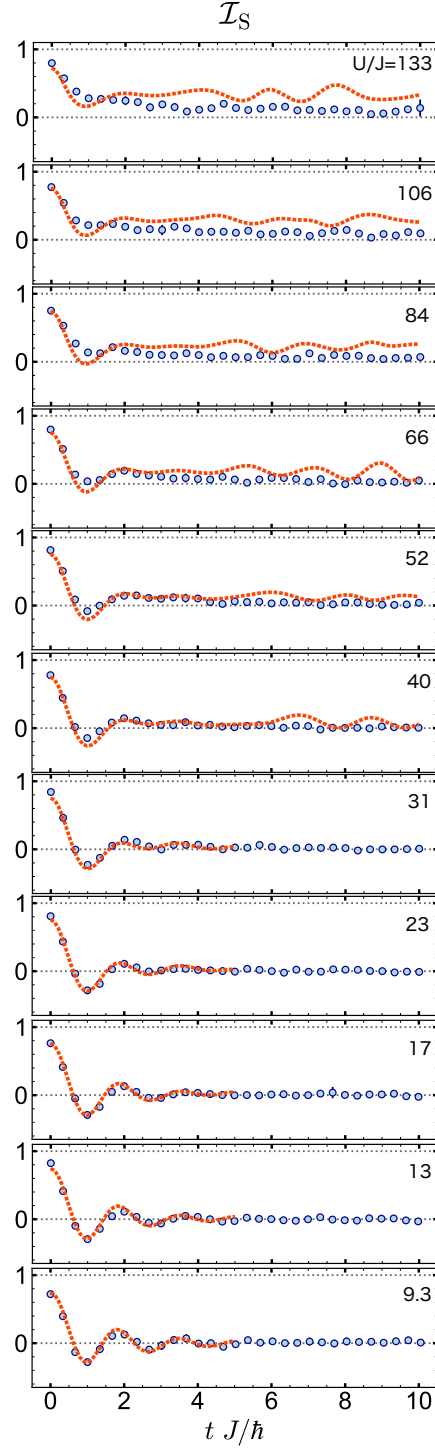


Figure 6.11: Systematic measurement of the quench dynamics from $\hat{\rho}_{\text{CDW(s)}}(0)$ state. The dependency of imbalance dynamics on U/J is shown. The horizontal axis shows the holding time normalized by the tunneling time for each lattice depth along the direction of the 1D chains. Error bars representing the standard deviation of five independent scans are smaller than symbols. The dotted curves show the calculated values. Error bars of the theory calculations represent the statistical error and are smaller than the dots of curves.

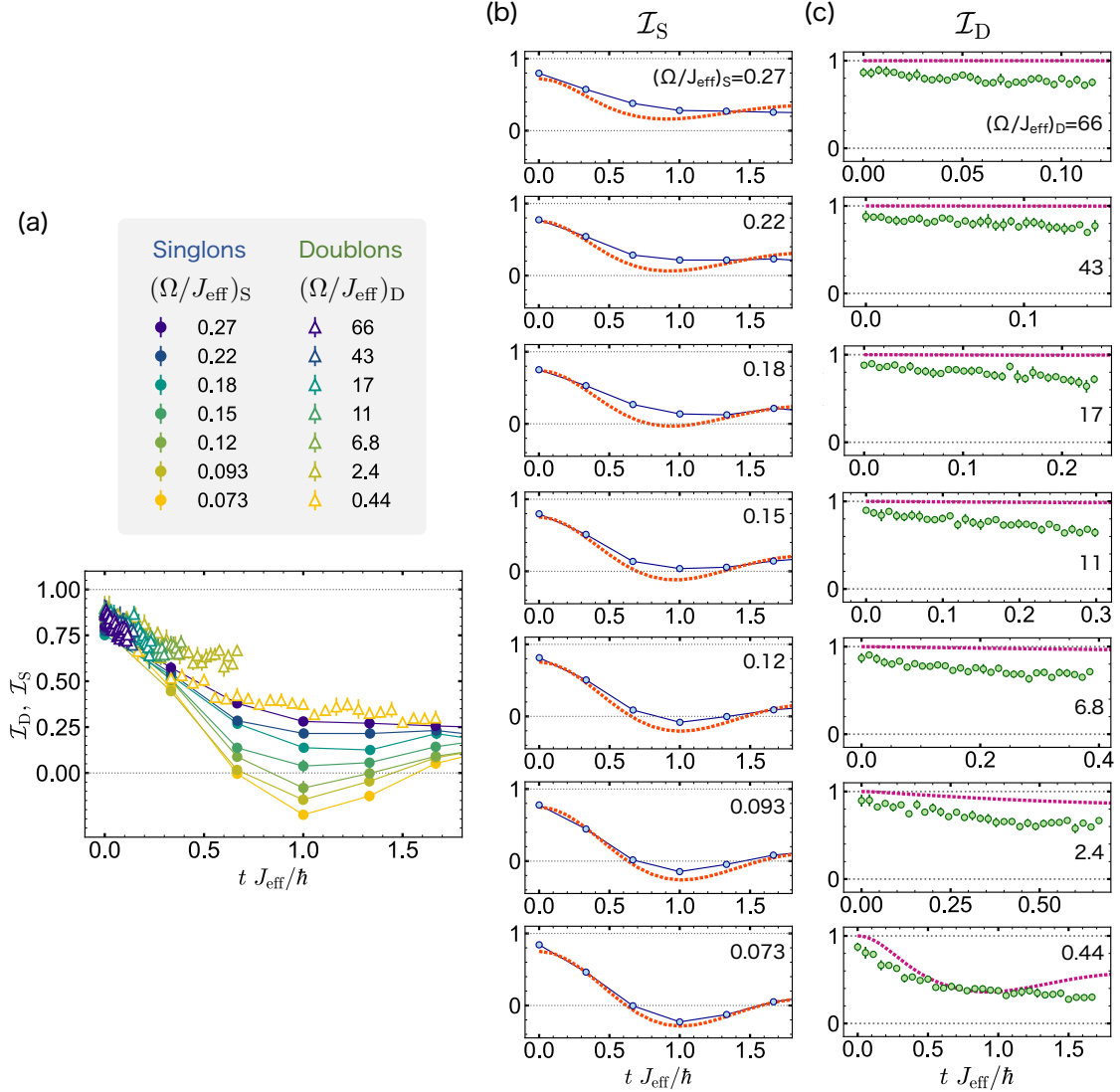


Figure 6.12: Comparison of the measured imbalance dynamics of singlons starting from $\hat{\rho}_{\text{CDW}(s)}(0)$ and those of doublons starting from $\hat{\rho}_{\text{CDW}(d,s)}(0)$ with the numerical calculations. (a) Systematically measured imbalance dynamics of singlons (solid circles) and doublons (open triangles) for various $(\Omega/J_{\text{eff}})_D$ and $(\Omega/J_{\text{eff}})_S$. The horizontal axis represents the normalized time by the effective tunneling amplitude J_{eff} , where $J_{\text{eff}} = J$ for singlons and $J_{\text{eff}} = 2J^2/U$ for doublons. (b), (c) Comparison of measured imbalance dynamics of (b) singlons and (c) doublons with the calculation for singlons (dotted curves) representing the case of non-interacting hardcore bosons. In the calculations of (b), the initial state is a mixed state $\hat{\rho}_{\text{CDW}(s)}(0)$ while in (a), it is a pure state $|\psi\rangle_{\text{CDW}(s)}(0)$. Error bars in (a)-(c) representing the standard deviation are mostly smaller than symbols.

s (E_R)	J/h (Hz)	U/J	Ω/J
5	266	9.3	0.027
6	206	13	0.035
7	160	17	0.045
8	125	23	0.058
9	98.2	31	0.073
10	77.7	40	0.093
11	61.9	52	0.12
12	49.6	66	0.15
13	40.0	84	0.18
14	32.4	106	0.22
15	26.4	133	0.27

Table 6.2: Bose-Hubbard parameters for the systematic measurement shown in Fig. 6.11.

$(\Omega/J_{\text{eff}})_S = \Omega/J$ $(\Omega/J_{\text{eff}})_D = (\Omega/J_{\text{eff}})_S \cdot (U/J)$, respectively. In Fig. 6.12, we show a comparison of the experimental results of the imbalance dynamics for the singlons for the initial $\hat{\rho}_{\text{CDW}(s)}(0)$ state and those for the doublon for the initial $\hat{\rho}_{\text{CDW}(d,s)}(0)$ state as a function of the time normalized by the effective tunneling amplitude J_{eff} . Note that, due to the large difference in the amplitude of J_{eff} between the singlons and doublons, the parameter regions of $(\Omega/J_{\text{eff}})_S$ and $(\Omega/J_{\text{eff}})_D$ have no overlap. Here, instead of the direct comparison of the experimental data, as shown in Fig. 6.12(c), we focus on the comparison of the experimental results for the doublons with the theoretical calculations for the singlons with the parameter region of $(\Omega/J_{\text{eff}})_S$ beyond 0.44 in accord with that for the doublons. Since the calculation for the singlons is rather straightforward, and indeed we see that the calculations well reproduce the experimental results for $(\Omega/J_{\text{eff}})_S$ below 0.23, as also shown in Fig. 6.11, we well expect the validity of the calculations for the singlons also for $(\Omega/J_{\text{eff}})_S$ beyond 0.44, which should be compared with the experimental results for the doublons in the corresponding region of $(\Omega/J_{\text{eff}})_D$. While the slow, non-oscillatory relaxation behavior is commonly observed both for the experiments and the calculations in Fig. 6.12(c), there is an overall discrepancy in that the experiments for the doublons show faster relaxation than the calculations. Note the effective parabolic trap strengths of $(\Omega/J_{\text{eff}})_S$ in the calculation and $(\Omega/J_{\text{eff}})_D$ in the experiments are the same in this comparison. The result of the comparison thus indicates that the doublons in this experiment cannot be simply interpreted as the non-interacting hardcore bosons, and we need to take interaction effects into consideration for full understanding of the observed behaviors.

First, we consider an effective nearest-neighbor doublon-doublon interaction, which is described in the following effective Hamiltonian for $U/J \gg 1$ [135]:

$$H^{\text{eff}} = \frac{2J^2}{U} \sum_{\langle i,j \rangle} \left[-8\hat{S}_i^z \hat{S}_j^z + \left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ \right) \right], \quad (6.15)$$

where the doublon and holon (empty site) are associated to a fictitious spin up $|\uparrow_i\rangle$ and down $|\downarrow_i\rangle$, respectively, and $\hat{S}_i^z \equiv (|\uparrow_i\rangle\langle\uparrow_i| - |\downarrow_i\rangle\langle\downarrow_i|)/2$ and $\hat{S}_i^+ \equiv |\uparrow_i\rangle\langle\downarrow_i| = (\hat{S}_i^-)^\dagger$ are the spin-1/2 operators. Here, the first term on the right-hand side corresponds to the doublon-doublon interaction, which takes the same order of magnitude as that of the second term for the doublon hopping. This doublon-doublon interaction introduces the energy difference between the state of doublons in the CDW and a state that possesses doublons occupying the nearest neighboring sites, causing the slower relaxation of the initially prepared CDW of the doublons compared with the case of non-interacting-hardcore bosons, in contrast to the observation in Fig. 6.12(c).

Next, we consider the interaction between the doublons and the singlons involved in the prepared initial $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state. See the situations depicted in Fig. 6.13(a). While the tunneling process of $|2,0\rangle \leftrightarrow |1,1\rangle$ is suppressed for $U \gg J$ as shown in Fig. 6.13(a) (left), that of $|2,1\rangle \leftrightarrow |1,2\rangle$, shown in Fig. 6.13(a) (right), has no energy cost, causing the faster relaxation of the initially prepared CDW of the doublons, consistent with the observation in Fig. 6.12(c). This behavior is also numerically confirmed as shown in Fig. 6.13(b), where we depict the time evolution of the atom density profile in a single Bose-Hubbard chain starting from the $|\psi(0)\rangle_{\text{CDW(d)}} = |\cdots 2020 \cdots\rangle$ state (left) and $\hat{a}_{\text{edge}}^\dagger |\psi(0)\rangle_{\text{CDW(d)}} = |\cdots 2020 \cdots\rangle$ (right). Here $\hat{a}_{\text{edge}}^\dagger$ creates an atom at a site $i_{\text{edge}} + 2$, where i_{edge} denotes the right-edge site of the initial doublon array. In the latter case, one singlon initially placed at the right edge of the trap moves to the trap center and disturbs $\cdots 2020 \cdots$ configuration, which leads to the significant decay of $I_D(t)$ as seen in the bottom panel of Fig. 6.13(b).

In order to experimentally confirm the effect of initially involved singlons on the quench dynamics, we prepare an initial $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state with a smaller singlon fraction by partially removing singlons with a selective ionization method, as depicted in Fig. 6.13(c). Specifically, we remove only singlons from a prepared $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state, which includes both doublons and singlons, by the excitation to the metastable 3P_2 state and subsequent ionization as follows (see Fig. 6.13(c), and also see Sec. 3.7 and Sec. 3.8 for the details of the excitation to the metastable 3P_2 state and subsequent ionization):

(1) Irradiate the atoms in the initial state $\hat{\rho}_{\text{CDW(d,s)}}(0)$ prepared in a 3D optical lattice of $40E_R$, where both doublons and singlons are involved, with an excitation laser resonant to the $^1S_0 \leftrightarrow ^3P_2$ ($m_J = 0$) transition at a wavelength of 507 nm. Here, we utilize a high-resolution laser spectroscopy with the well-separated resonance frequencies for singlons and doublons resulting from the on-site interaction shift of the resonance frequency associated with doublons, enabling us to excite only singlons to the metastable state [58, 210, 189].

(2) Irradiate the atoms with a laser beam at a wavelength of 325 nm, which induces a single-photon ionization for the metastable 3P_2 state. Note that we observe a loss of atoms

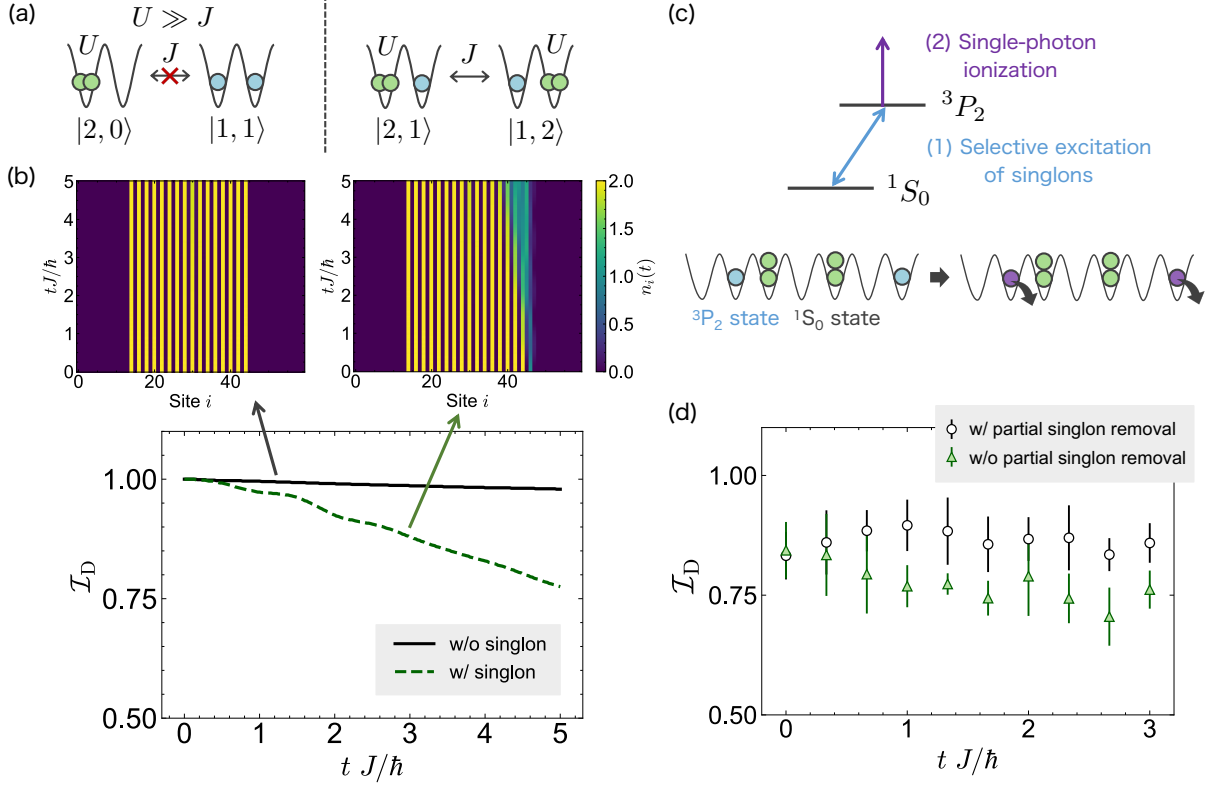


Figure 6.13: Effect of singlons on the imbalance dynamics. (a) Schematic illustration of possible tunneling processes involving singlons between nearest-neighbor sites. (b) Calculated time evolution of the local density in the 1D Bose Hubbard model (Eq. (6.9)) for $U/J = 52$, starting from $|\psi(0)\rangle_{\text{CDW(d)}} = |\cdots 2020 \cdots\rangle$ state (upper left) and $\hat{a}_{\text{edge}}^\dagger |\psi(0)\rangle_{\text{CDW(d)}}$ state (upper right), where one singlon is placed at the right edge of the trap in this case. (lower) Imbalance dynamics of doublons ($\mathcal{I}_D$) obtained from the data in (upper). (c) Schematic illustration of the removal procedure of only singlons from the initial $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state and the relevant energy levels. (d) Imbalance dynamics of doublons after partial removal of singlons in the initial $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state. Here, the plots of the open circle and solid triangle show the results with ($n_s = 0.24$) and without ($n_s = 0.29$) partial removal of singlons, respectively. Note that the loss of doublons in this measurement is negligibly small within the uncertainty. Both data are obtained at $U/J = 52$. All error bars show the standard deviation.

in the 3P_2 state at a rate of about 3.0 kHz for the intensity of a 325 nm laser of 23 W/cm², as also described in Sec. 3.8.

In Fig. 6.13(d), we show the imbalance dynamics of doublons starting from a $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state with and without the partial singlon removal as the open circle and the solid triangle, respectively. Note that by the above scheme, we could not achieve a complete removal of singlons but only achieve a partial removal of singlons in a prepared $\hat{\rho}_{\text{CDW(d,s)}}(0)$ state, although we also try the iteration of the above removal scheme. Note that when we perform several iterations of the above removal scheme, we observe non-negligible losses also in doublons. Although the complete removal of singlons in the initial state is not achieved in this work, we importantly observe the slower relaxation of the imbalance of doublons in the case of a smaller singlon fraction in the initial state. In this way, we confirm the novel role of initially involved singlons in the quench dynamics, which qualitatively agrees with the numerical result.

6.3 Summary and outlook

In summary, we experimentally studied nonequilibrium dynamics of 1D Bose gases in optical lattices, which is well described as 2D arrays of independent Bose-Hubbard chains, after a sudden quench of the optical lattice depth. Starting from an initial period-two CDW state of doublons slightly mixed with singlons, we successfully observed slow relaxation in an imbalance measurement. We found that the numbers of both doublons and singlons are almost conserved during the dynamics, which strongly supports the occurrence of HSF. Systematic measurements of quench dynamics for various U/J and the quantitative comparison of measured and calculated dynamics were also performed. In addition, we revealed the effect of singlons involved in the initial $|\cdots 2020 \cdots\rangle$ state on the quench dynamics.

The successful preparation of arrays of dense doublons, i.e., $|\cdots 2020 \cdots\rangle$ state, and observations of dynamics of interacting doublons with a long lifetime open the possibility to study systems consisting of strongly-interacting composite particles with ultracold gases. For instance, it is interesting to examine whether some exotic quantum many-body states formed by such composites can be experimentally realized, such as the pair superfluids of bosons [211], the η -pairing state [212], and quantum many-body scar states [121, 122].

CONCLUSION & OUTLOOK

In this thesis, we performed three optical lattice experiments. Here, we briefly review the achievements in each work and present some future outlooks.

- *Exploring the Strongly-Interacting Regime of Effective Multi-Body Interactions in a Trapped Ultracold Atom System* (Chapter 4)

We investigated a few-body system comprising of ultracold bosons tightly confined in a deep optical lattice site, which is effectively described as zero-dimensional bosons. By combining an occupancy-resolving high-resolution laser spectroscopy with an inter-orbital Feshbach resonance controlling the bare two-body interaction over a wide range, we experimentally revealed the behaviors of few-atom systems in a strongly-interacting regime. Our results, for which perturbative calculations do not provide proper explanations, serve as a valuable and precise benchmark for theoretical approaches to strongly interacting few-body systems. As one important illustration, we obtained a clear signature of an effective four-body interaction, evidenced by the binding energies of more than four atoms.

As an outlook, it is instructive to consider this injected few-body state in the context of the Bose polaron problem, which may provide an indispensable viewpoint for this system. Also, it is straightforward to apply the same methodology to study strongly-interacting regime of spinful atoms of both fermions and bosons, and also with long-range dipolar interactions provided by magnetic atoms and molecules or Rydberg atoms. Systematic investigations of these various systems would provide important insights into, for example, how the few-body limit can illuminate the quantum many-body problem by taking larger values of the number of atoms, which may provide a possible relation to a strongly-interacting bosonic liquid.

- *Observation of the sign reversal of the magnetic correlation in a driven-dissipative fermi gas in double wells.* (Chapter 5)

We studied quantum magnetism in a dissipative Fermi-Hubbard system with on-site two-body losses, which was introduced in a controlled manner utilizing a PA technique. Here, we successfully observed the sign reversal of the magnetic correlation from antiferromagnetic to ferromagnetic, which had been theoretically predicted. We systematically measured the dynamics of the nearest-neighbor spin correlation in an isolated double-well optical lattice, as well as a crossover from an isolated double-well lattice to a one-dimensional uniform lattice. In a wide range of lattice configurations over an isolated double-well lattice, we observed a ferromagnetic spin correlation, which is consistent with a Dicke type of correlation expected in the long-time limit. This work demonstrates the control of quantum magnetism in open quantum systems with dissipation.

As a future outlook, a quantum gas microscope (QGM) is expected to directly observe the effect of the dissipation on the long-range magnetic correlation due to the spin-charge separation in a 1D uniform lattice and its dynamics [213, 214]. A QGM may also allow us to observe the dissipation-induced spin-charge separation in a 1D uniform lattice, which has been theoretically predicted [215]. In higher dimensions (2D and 3D), the spin-charge separation does not occur. Thus, the behavior of the long-range magnetic correlation in a dissipative 2D or 3D system is an interesting problem. Moreover, the reversal of the magnetic correlation is also predicted for a bosonic system [84]. By utilizing the 3P_2 state of ^{174}Yb , which has the spin degrees of freedom and intrinsic inelastic interaction between them [80], the reversal may be experimentally observed.

- *Observation of slow relaxation due to Hilbert space fragmentation in strongly interacting Bose-Hubbard chains.* (Chapter 6)

We experimentally studied nonequilibrium dynamics of 1D Bose gases in optical lattices, which is well described as 2D arrays of independent Bose-Hubbard chains, after a sudden quench of the optical lattice depth. Starting from an initial period-two CDW state of doublons slightly mixed with singlons, we successfully observed slow relaxation in an imbalance measurement. We found that the numbers of both doublons and singlons are almost conserved during the dynamics, which strongly supports the occurrence of HSF. Systematic measurements of quench dynamics for various U/J and the quantitative comparison of measured and calculated dynamics were also performed. In addition, we revealed the effect of singlons involved in the initial $|\cdots 2020 \cdots\rangle$ state on the quench dynamics.

As an outlook, it is interesting to examine whether some exotic quantum many-body states formed by strongly-interacting composite particles with ultracold gases can be

experimentally realized, such as the pair superfluids of bosons [211], the η -pairing state [212], and quantum many-body scar states [121, 122].

JOURNAL ARTICLES

Below is the list of journal articles to which I contributed during this course.

- *Observation of the sign reversal of the magnetic correlation in a driven-dissipative fermi gas in double wells.*

K. Honda, S. Taie, Y. Takasu, N. Nishizawa, M. Nakagawa, and Y. Takahashi,
Phys. Rev. Lett. **130**, 063001 (2023).

- *Exploring the Strongly-Interacting Regime of Effective Multi-Body Interactions in a Trapped Ultracold Atom System.*

K. Honda, Y. Takasu, Y. Haruna, Y. Nishida, and Y. Takahashi,
arXiv:2402.16254v2 (2024).

- *Observation of slow relaxation due to Hilbert space fragmentation in strongly interacting Bose-Hubbard chains.*

K. Honda, Y. Takasu, S. Goto, H. Kazuta, M. Kunimi, I. Danshita, and Y. Takahashi.

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