Quantum simulation of interaction blockade in a two-site Bose–Hubbard system with solid quadrupolar crystal

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Abstract

The Bose–Hubbard model provides an excellent platform for exploring exotic quantum coherence. Interaction blockade is an important fundamental phenomenon in the two-site Bose–Hubbard system (BHS), which gives a full quantum description for the atomic Bose–Josephson junction. Using the analogy between the two-site BHS and the quadrupolar nuclear magnetic resonance (NMR) crystal, we experimentally simulate a two-site Bose–Hubbard system in a NMR quantum simulator composed of the quadrupolar spin-3/2 sodium nuclei of a NaNO\textsubscript{3} single crystal, and observe the interesting phenomenon of interaction blockade via adiabatic dynamics control. To our best knowledge, this is the first experimental implementation of the quantum simulation of the interaction blockade using quadrupolar nuclear system. Our work exhibits important applications of quadrupolar NMR in the quantum information science, i.e. a spin-3/2 system can be used as a full 2-qubit su(4) system, if the quadrupole moment is not fully averaged out by fast tumbling in the liquid phase.

1. Introduction

The simulation of physical phenomena in many-body quantum systems using a controllable quantum system, called quantum simulation, has attracted extensive research interest since Richard Feynman’s idea in 1982 [1]. Various physical systems for implementing quantum simulation have been proposed, including nuclear magnetic resonance (NMR) [2], trapped ions [3], and quantum dots [4] (also see a recent review on quantum simulation [5]). Among these NMR is one of the most well-developed architectures. Plenty of relevant experimental research has been done on the platform, such as simulating quantum phase transition in condensed matter physics [6] and quantum chemistry [7].

Most of the quantum simulation experiments have been carried out on the spin-1/2 nuclei so far, where each nucleus represents a qubit and the spin–spin interactions are used to realize the nonlocal quantum gates. In contrast, one quadrupolar nucleus can be encoded as more than one qubit due to its multi-level property, for example, a spin-3/2 nucleus can be used as a 2-qubit system. At the same time, the quadrupolar coupling as large as several MHz results in a fast control over the system, as well as the possibility to implement quantum information processing without strong external static magnetic fields by the technology of nuclear quadrupolar resonance (NQR) [8, 9]. Moreover, the nonlinear Hamiltonian in the quadrupolar nuclei whose spin number \( I > 1/2 \) provides a perfect workbench of analog quantum simulation [5] (AQS) for nonlinear quantum systems which are more difficult to be simulated with spin-1/2 nuclei, such as the Bose–Hubbard system (BHS) and quantum chaotic systems. Consequently, the quadrupolar NMR quantum information processing has already
attracted the interest of researchers [10, 11]. Several basic experiments have been done in recent years, including the pseudo-pure state preparation [12], quantum state tomography [13], relaxation study [14], quantum algorithms [15] and some quantum simulation experiments [16, 17]. In contrast to the systems with the spin-1/2 nuclei, the main obstacles of using quadrupolar nuclei as quantum information processors are as follows: firstly, the higher spin quantum number results in more energy levels, which makes the operations more difficult; secondly, the first-order quadrupolar Hamiltonian exists only in the solid and liquid crystalline states for the first-order quadrupolar coupling dynamically averaged to zero in the liquid states, which usually results in shorter decoherence times [18]; finally, the dipolar coupling between different quadrupolar nuclei is usually small which is a challenge for its scalability.

As a typical many-body quantum system, Bose–Einstein condensate (BEC) has attracted interests since it was predicted by Bose and Einstein in 1924. The first BEC was realized by using ultracold rubidium atomic gases [19]. The Bose–Hubbard model (BHM), first introduced by Fisher et al [20], describes cold atoms in an optical lattice at finite density. The experimental realization of quantum phase transition between superfluid and Mott-insulator were first observed by Greiner [21] and then by Stoferle [22] and Spielman [23]. The Bose–Josephson system (BJS), a system of two BECs linked by Josephson coupling [24, 25], which can be quantum described fully by the two-site BHM, has been widely used to explore and exploit exotic quantum coherence, such as macroscopic quantum coherence [26], Josephson effects [27], decoherence [28], many-body quantum interferometry [29], mesoscopic entangled states [30], the Kibble–Zurek mechanism [31], nonlinear Landau–Zener tunneling [32, 33], coherent destruction of tunneling [34], and interaction blockade [35, 36]. There are two types of experimental methods to realize a two-site BHS with ultracold atoms: (i) loading Bose condensed atoms in a single double-well potential [37–39], and (ii) loading Bose condensed atoms in double-well lattices with several double-well subsystems [40–42]. In the first method, the total particle number is difficult to control accurately, and it is difficult to reach the single-particle level using the measurement process. In the second method, one has to average all double-well subsystems and each subsystem may have different total particle numbers. Given the importance and the difficulties of implementing the two-site BHS, it is of great significance to simulate it with another quantum system that is easier to control. The quadrupolar nuclei NMR system proves to be a good candidate. Using a spin-1 (> 1/2) quadrupolar nucleus, one can, in principle, simulate a two-site BHS with a total particle number \( N = 2J \). However, the total particle number \( N \) that can be simulated is practically limited by the highest nuclear spin \( J \) of a natural quadrupolar isotope nucleus in the entire periodic table (e.g. \( J = 7 \) for \(^{176}\)Lu) [43]. As a substitute, the single molecular magnet (a macroscopic quantum system) has a high spin ground state (e.g. \( J = 37 \) in [\( \text{Mn}
\)\(_{12} \) complexes [44]), a big zero-field-splitting and negligible magnetic interaction between molecules. Additionally, the Bose–Hubbard model with more than two sites may be simulated with a dipolar-coupled quadrupolar nuclei system.

Some related work has been done before, e.g. simulating the propagation of excitation along a one-dimensional chain of atoms [16], and a BEC system [17], where only a time-independent target Hamiltonian was simulated using quadrupolar NMR systems. In this paper, we present a dynamic simulation of a time-dependent Hamiltonian for atomic BHS in a solid quadrupolar NMR quantum simulator by adiabatic control, in which the interaction blockade in the atomic BJS was observed. The article is organized as follows: in section 2, we investigate the analogy of the atomic BHS and the quadrupolar NMR system; in section 3, we describe our NMR experiment of simulating the dynamics of the BHS; in section 4, some conclusions and discussions are presented.

2. Analogy between atomic Bose–Hubbard system and solid quadrupolar crystal

2.1. Atomic Bose–Hubbard system

The Hamiltonian of a two-site BHS can be described as,

\[
H_{BH} = J \left( a_1^\dagger a_2 + a_1 a_2^\dagger \right) + \frac{\delta}{2} (n_2 - n_1) + \frac{E_c}{8} (n_2 - n_1)^2. \tag{1}
\]

Here, \( a_j, (a_j^\dagger), n_j = a_j^\dagger a_j \) (\( j = 1, 2 \)) are the particle annihilation (creation) operators and the particle number operators of the \( j \)th site, \( J \) is the inter-site tunneling strength, \( \delta \) is the asymmetry between the two sites, and \( E_c \) describes the nonlinear inter-particle interaction. The above BHS conserves the total particle number \( N = n_1 + n_2 \). Under the condition of weak tunneling (\( |J| \ll |E_c| \)) and positive nonlinearity (\( E_c > 0 \)), we consider the asymmetric system (i.e. \( \delta \neq 0 \)). For the case of the large total particle number, the above Hamiltonian gives a full quantum description for the atomic Bose–Josephson systems [24, 25].

The energy-level structure for the system with \( N = 3 \) and \( J/E_c = 0.02 \) is shown in figure 1(a). The notation in the bracket shows the four eigenstates of the system in the representation of Fock states \( |n_1, n_2\rangle \), which means that there are \( n_1 \) particles in the first site and \( n_2 \) in the second site, and the total particle number \( N = 3 \) is conserved. The degeneracy points (denoted as A, B, C, D, E and F) are opened when \( J \) is nonzero, which results in

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single-atom tunneling in A, B and C, two-atom tunneling in D and E, and three-atom tunneling in F. When $J/E_C \ll 1$, the ground state $|\psi_g\rangle$ is determined by the ratio $\delta/E_c$,

$$
|\psi_g\rangle \approx \begin{cases} 
|3, 0\rangle & \frac{\delta}{E_c} < -1.0 \\
|2, 1\rangle & -1.0 < \frac{\delta}{E_c} < 0 \\
|1, 2\rangle & 0 < \frac{\delta}{E_c} < 1.0 \\
|0, 3\rangle & \frac{\delta}{E_c} > 1.0.
\end{cases}
$$

Near the critical points A, B, and C, the ground state is a linear superposition of the two neighbor Fock states, $|\psi_g\rangle = a|n_1, n_2\rangle + b|n_1 - 1, n_2 + 1\rangle$. Therefore, by changing the value of $\delta$ while keeping the system in its ground state, we can control the dynamics of single-atom tunneling which takes place in the vicinity of A, B, and C. This can be demonstrated with the technique of adiabatic control. The time-evolution of the half relative particle number of the two sites $N_f/2 = (n_1 - n_2)/2$ is shown in figure 1(b).

The regular plateaus and the sudden steps represent the interaction blockades and the single-atom resonant tunnelings in the BHS respectively [35]. Figure 1(c) shows the instantaneous ground states of the BHS as we change $\delta$ from $-1.5E_c$ to $1.5E_c$; we see that the ground state of the system gradually transfers from $|3, 0\rangle$ to $|0, 3\rangle$.

### 2.2. Solid quadrupolar NMR system

For a quadrupolar NMR system, the Hamiltonian [43],

$$
H_{\text{NMR}} = H_z + H_Q + H_{rf},
$$

consists of three contributions: the Zeeman term $H_z$, the quadrupolar term $H_Q$ and the radio-frequency (RF) field term $H_{rf}$. If the static magnetic field $B_0$ is oriented in the $z$-direction, one has $H_z = -\gamma B_0 I_z$, where $\gamma$ is the gyromagnetic ratio of the nucleus, and $I_\alpha$ ($\alpha = x, y, z$) is the spin angular momentum of a spin-$I$ nucleus. The quadrupolar term $H_Q$ describes the interaction of the nuclear quadrupolar moment and the electric field gradients (EFG) generated by the surrounding charge distribution and it can be written as $H_Q = \frac{\alpha I}{2(2I-1)} \mathbf{V}(\Theta) \mathbf{I}$, where $\mathbf{I} = (I_x, I_y, I_z)$, $Q$ is the quadrupolar moment, and $\mathbf{V}(\Theta)$ is a second-order tensor describing the EFG with $\Theta$ the Euler angle of the molecule. Under the condition of the high field, i.e. the Zeeman interaction is much stronger than the quadrupolar interaction (in our case $\omega_0/\omega_Q \sim 1.27 \times 10^6$), where the secular approximation is satisfied, the first-order quadrupolar Hamiltonian $H_Q^{(1)} = \omega_0 (3I_z^2/2 - I(I+1)) + \eta (I_x^2 - I_y^2)$ is sufficient to

![Figure 1. (a) Energy level diagram of two-site Bose–Hubbard Hamiltonian with $E_r = 83.4$ kHz, $J = 1668$ Hz. The degeneracies at points A, B, C, D and E are eliminated when a nonzero $J$ is introduced. (b) Half relative atom number versus the asymmetry $\delta$. (c) Illustration of the single-atom tunneling dynamics. The balls represent the atoms in two different sites.](image)
describe the interaction. Here $I$ is the identity matrix, $\omega_Q = \frac{3\gamma V_{q} Q}{4I(I+1)} (3 \cos^2 \theta - 1)$ is the quadrupolar coupling, $V_{q} Q$ is the $z$-component EFG in the principal axis system (PAS), $\eta = -\frac{V_{q} Q}{V_{q} c}$ the asymmetry of the EFG, and $\theta$ the angle between the $z$-axes of the PAS and laboratory frame. The RF field term reads as $H_{rf} = -\gamma B_{1z} (I_x \cos(\omega_{rf} t + \phi) + I_y \sin(\omega_{rf} t + \phi))$, which is induced by the interaction of nuclear spin magnetic momentum and the RF field aligned perpendicularly to the static magnetic field. $B_{1z}$, $\omega_{rf}$ and $\phi$ are the amplitude, frequency and phase of the RF field, respectively.

If $\phi = 0$ and the EFG is axial symmetric (i.e. $\eta = 0$), the whole Hamiltonian of the quadrupolar nuclear system in the rotating frame of frequency $\omega_{rf}$ is

$$H_{\text{NMR}} = \frac{\omega_0}{6} (3 I_z^2 - I (I + 1)) + (\omega_0 - \omega_{rf}) I_z + \omega_{rf} I_x,$$

where $\omega_0 = -\gamma B_0$ is the Lamor frequency of the nuclei, and $\omega_0 = -\gamma B_1$ represents the nutation frequency resulting from the RF field. In isotropic liquids, the quadrupolar coupling will be averaged out because of the molecular rapid tumbling. Therefore the quadrupolar interaction will not influence the energy structure but significantly influence the relaxation of the system. While in liquid crystals and solids, the quadrupolar coupling can not be motionally averaged out, i.e. $\omega_Q \neq 0$ [43]. In polycrystalline powders, there is a distribution of $\omega_Q$ due to the anisotropy of the molecules, and in single crystals, $\omega_Q$ can be tuned by changing $\theta$.

2.3. Analogy between BHS and quadrupolar crystal

By expressing the angular momentum operators in the Schwinger representation [45]

$$I_x = \frac{a_1^+ a_2 + a_2^+ a_1}{2}, \quad I_y = \frac{i(a_1^+ a_2 - a_2^+ a_1)}{2}, \quad I_z = \frac{a_1^+ a_2 - a_2^+ a_1}{2},$$

the Hamiltonian (6) can be rewritten as

$$H_{\text{NMR}} = \frac{\omega_0}{2} (a_1^+ a_2 + a_2^+ a_1) + \frac{\omega_0 - \omega_{rf}}{2} (n_2 - n_1) + \frac{\omega_Q}{8} (n_2 - n_1)^2.$$  

Here $n_j = a_j^+ a_j$ ($j = 1, 2$) is the particle number of the $j$th site, then the total and the relative particle number can be represented as $N = n_1 + n_2$, $N_r = n_2 - n_1$. The part $\frac{\omega_0}{6} I(I + 1)$ proportional to the identity matrix is neglected. Comparing equation (6) to equation (1), we can see the similarity between the quadrupolar NMR Hamiltonian and the two-site BHS. This allows us to simulate the two-site BHS with the quadrupolar NMR system analogously. To achieve the equivalence between the two systems, the coefficients should satisfy

$$\frac{\omega_0}{2} = \frac{\omega_0 - \omega_{rf}}{\delta} = \frac{\omega_Q}{E_c}.$$  

(7)

Obviously, one can easily find that the nutation frequency $\omega_0$, offset $\omega_0 - \omega_{rf}$, and quadrupolar coupling $\omega_Q$ in the quadrupolar NMR system play the roles of the inter-mode tunneling strength $J$, the asymmetry parameter $\delta$ and the nonlinear interaction $E_c$ in the BHS respectively. And the half relative number $N_r/2$ of the BHS corresponds to the magnetization in $z$-direction $M_z$ in the NMR system, the total particle number $N$ equals the maximum relative particle, i.e. $N = \max(N_r)$. A spin $-I$ quadrupolar nuclei can be mapped to a $N = 2I$ two-site BHS.

To simulate two-site Bose–Hubbard Hamiltonian with a quadrupolar NMR system, it is necessary to match their time evolution in such a way that the propagator $V(t) = \exp(-iH_{\text{NMR}} t_{\text{NMR}})$ equals $U(t) = \exp(-iH_{Bij} t_{Bij})$. If equation (7) is satisfied, we only have to set

$$\frac{t_{\text{NMR}}}{t_{Bij}} = \frac{E_c}{\omega_Q}.$$  

(8)

Accordingly, the dynamics of the atomic BHS can be analogously simulated with an ensemble of single-NMR quadrupolar nuclei.

3. Experimental observation

The experiment was carried out on a Bruker AVANCE-III 400 spectrometer (9.4 T) at room temperature. The NMR quadrupolar system we used is the $^{23}$Na ($I = 3/2$) nuclei in NaNO$_3$ single crystal with a size of about $4 \times 4 \times 1$ mm$^3$, obtained by slow evaporation of a water solution at room temperature. The crystal structure [46] and the relevant parameters are shown in figure 2(a). The sample, fixed in a 5mm NMR tube, was oriented to a Bruker TBO probehead in such a way that the quadrupolar coupling constant was about $\omega_Q = 83.4$ KHz with resonance frequency 105.84 MHz. The large quadrupolar coupling allows us to manipulate the system faster than liquid-state systems and at the same time keeps the decoherence effect reasonably small. We
measured the relaxation parameters using the same method proposed by Auccaise [14] as illustrated in figure 2(a). In our system, the longitudinal relaxation time $T_1$ is four orders larger than the transverse relaxation time $T_2$, i.e. $T_1 \gg T_2$. Compared to liquid crystal quadrupolar NMR samples presented in previous research [12], the single-crystal one has the following merits: it is more stable in physics and less sensitive to the temperature fluctuation; the quadrupolar coupling is always larger because of the stronger electrical gradient field [47], which leads to a faster coherence operation time; the quadrupolar coupling is adjustable in a large range by changing sample orientation $\theta$ in the static magnetic field. A disadvantage of the solid-state system is that the decoherence time will also be shorter than a liquid crystal.

The experiment consists of three parts: initial state preparation, dynamical evolution and readout, as schematically shown in figure 2(b). The spin $I = \frac{3}{2}$ nucleus allows us to simulate a three-particle BHS.

### 3.1. Initial state preparation

The thermal equilibrium state of a spin-$I$ quadrupolar NMR system can be written as

$$\rho_0 \approx \frac{1}{2I+1} \mathbb{I} + \epsilon I_z,$$

(9)

where $\epsilon = \frac{\gamma R}{k_B T}$ is the polarization ($\sim 10^{-6}$) and $k_B$ is the Boltzmann constant. When we sweep the asymmetry $\delta$ from $-1.5E_c$ to $1.5E_c$, the initial state $|\psi_0 (\pm 1.5)\rangle$, corresponding to the ground state at the point $\delta/E_c = -1.5$, is approximately the Fock state $|3, 0\rangle$, as denoted by equation (2). The theoretical fidelity $|\langle\psi_0 |(-1.5)|3, 0\rangle|$ between the initial state and the Fock state is 99.5% for $J/E_c = 0.02$ and 98.2% for $J/E_c = 0.04$. In the NMR system, we can initialize the system into a pseudo-pure state $\rho_{pp} = \frac{1-\epsilon}{2I+1} I_z + \epsilon |3, 0\rangle \langle 3, 0|$, which can be equivalent to the pure state $|3, 0\rangle$ [48].

To initialize the system to the PPS $\rho_{pp}$ from the thermal state $\rho_0$, a shaped radio-frequency pulse searched by the gradient ascent pulse engineering (GRAPE) algorithm [49] was used to equalize populations of three among the four energy levels; then a phase cycling was utilized to remove the coherence terms so that only the diagonal terms remained [51]. The GRAPE pulse is of a length of 180 $\mu$s consisting of 90 segments of different phases and amplitudes, with the theoretical fidelity above 99.9%.

### 3.2. Adiabatic dynamical evolution

To observe the dynamical evolution shown in figure 1(b), the system must always stay on the ground state of the time-dependent Hamiltonian. This was achieved by the quantum adiabatic dynamical evolution, which
guarantees a high fidelity between the system state and its instantaneous ground state when the following three conditions are satisfied: (i) the system starts from an initial ground state; (ii) there is no level-crossing between this ground-state energy level and the others; (iii) the time-dependent Hamiltonian \( H(t) \) has to change slowly enough to satisfy the quantum adiabatic condition \([52]\):

\[
\frac{d\delta(t)}{dt} = \chi \left| \frac{(e_{ic} - e_{e})^2}{\langle \psi_{ic} | \partial \delta H | \psi_{eg} \rangle} \right|.
\]

Here \( \chi \) is a constant adiabaticity parameter which satisfies \( \chi \ll 1 \), \( e_{e} \) and \( e_{ic} \) are the energies of the ground state \( |\psi_{g} \rangle \) and the first excited state \( |\psi_{eg} \rangle \) of \( H(t) \). Equation (10) determines the sweep speed of \( \delta(t) \) during the dynamical evolution. The solid line in figure 3(a) shows how \( \delta(t) \) can change with time \( t \) from \(-1.5E_{c}\) to \(1.5E_{c}\) to keep a constant \( \chi \).

The dynamical evolution was accomplished by adiabatically changing the RF field frequency offset \( \omega_{0} - \omega_{rf} = \delta \) from \(-1.5E_{c}\) to \(1.5E_{c}\). And the continuous varying of time-dependent \( \delta(t) \) was discretized into \( M+1 \)-segment discrete-time \( \delta(m) \) with \( \delta(0) = 0 \) and \( \delta(M) = \delta(T) \). Then the corresponding continuous varying of time-dependent Hamiltonian \( H(t) \) was discretized into \( M + 1 \)-segment discrete-time Hamiltonian \( H[m] \) with \( H[0] = H[\delta(0)] \) and \( H[M] = H[\delta(T)] \) so that \( H[m] = s(m/M) H[0] + (1 - s(m/M)) H[M] \), where \( s(m/M) \) is the interpolation function and satisfies \( 0 \leq s(m/M) \leq 1 \). The dynamical evolution can be written as

\[
U = \prod_{m=0}^{M} U_{m} = \prod_{m=0}^{M} e^{-iH[m] \Delta t},
\]

where the duration of each segment is \( \Delta t = T/(M + 1) \). The adiabatic condition corresponds to \( T, M \to \infty, \Delta t \to 0 \). We used a numerical optimization procedure to determine \( M \) and \( T \). We numerically calculated the average state fidelities \( F_{avg}(M) = \langle \psi_{eg} | \langle \psi_{eg} \rangle \rangle \) during the dynamical evolution, where \( |\psi_{eg}(K)\rangle \) is the ideal ground state of the \( K \)-th segment Hamiltonian \( H[K] \). As shown in figure 3(b), \( F_{avg}(M) \) will approach 1 asymptotically as the number of steps increases in the case of no relaxation. However, due to the relaxation effect in practical experiments, we can find an optimal scan step number \( M_{opt} \approx 50 \) with \( \chi = 0.216 \) in our studied system when \( J|E_{c}| = 0.02 \). Here, we only consider the transverse relaxation \( T_{2} \) due to the fact that \( T_{2} \gg T_{1} \). In the experiment, we chose \( M = 40 \) with \( \chi = 0.269 \) (the fewer steps but a slightly low fidelity close to the optimal point \( M_{opt} \approx 50 \)). The red circles in figure 3(a) denote the values used in experiment in \( M + 1 = 41 \) steps.

In the experiment, instead of directly varying the RF pulse frequency offset, we used a sequence of phase-incremented pulses \([50]\), that is, by varying the phase of the RF pulse to achieve the same goal. In the on-
resonance case, i.e. \( J_{\phi} = \omega_0 \), the Hamiltonian of a single quadrupolar spin in the rotating frame whose frequency reference to the laboratory is the Larmor frequency \( \omega_0 \) can be written as

\[
H_{\text{NMR}} = \frac{\alpha_J}{\delta} \left( 3I_z^2 - I(I+1)I \right) + \omega_1 \left( I_x \cos \phi + I_y \sin \phi \right).
\]  

(12)

When the phase \( \phi \) changes linearly with time as \( \phi(t) = -\delta t \), then in the rotating frame \( \omega_0 = \delta \), the effective Hamiltonian is in the same form as equation (4) with \( \delta = \alpha_J - \alpha_{\phi} \). This is the so-called phase-incremented pulse. In practice, the continuous linear phase shift \( \phi(t) \) is realized with \( L \) discretized rectangular pulses of the same duration \( dt = \Delta t/L \) and amplitude \( \omega_1 \). The phase increment of each two sequential rectangular pulses is \( \Delta \phi = -\delta [m] \) dr if we want a frequency shift of \( \delta [m] \). To implement the whole adiabatic evolution, the initial phase of the \( K \)th-segment pulse changes with time as \( \phi [K] = \sum_{m=0}^{K-1} \delta [m] \Delta t \) as illustrated in figure 2(b), and the global phase generated by this method does not affect the readout of the diagonal terms.

3.3. Readout

The dynamics of quantum tunneling can be observed by complete quantum state tomography [13]. Here we only measured the longitudinal magnetization \( \langle M_z(K) \rangle = \langle \psi_f(K) | I_z | \psi_f(K) \rangle \) = \( \langle \psi_f(0) | \prod_{m=0}^{K} U_{m} | \psi_f(0) \rangle \) where \( K \) corresponds to the half relative particle number \( N_r/2 \) of the BHS. In NMR, \( \langle M_z(K) \rangle \) was measured by observing the signal in the \( x \)-direction after applying a \( \pi/2 \) pulse along the \( y \)-direction. The readout pulse was optimized with the GRAPE method, and phase cycling was used to select the population terms of the density matrix. Figure 4 shows the measured values \( \langle N_r \rangle/2 \) (denoted by the crosses) as a function of \( \delta [E_c] \) for two different inter-well tunneling strengths \( J \), i.e. \( J/E_c = 0.02 \) and 0.04. The plateaus and the sudden transitions representing the interaction blockades and single-atom tunnelings are obviously observed in the neighbourhoods of A, B and C. The dashed lines are the theoretical expectations calculated with the ideal ground states \( |\psi_f(\tau)\rangle \) of the instantaneous Hamiltonian \( H(\tau) \), and the solid lines denote the simulated results with decoherence. In the experiments, the optimal parameters of \( T = 290 \mu s, M = 40 \) when \( J/E_c = 0.02 \), and \( T = 175 \mu s, M = 50 \) when \( J/E_c = 0.04 \) were used. As the larger \( J/E_c \) leads to the larger energy gap, the total evolution time is relatively shorter in the case of \( J/E_c = 0.04 \) than that in the case of \( J/E_c = 0.02 \). From figure 4, it can also be seen that in the weak tunneling case, the relatively smaller \( J/E_c \) results in the sharper transitions and the wider plateaus. Thus we can conclude that the interaction blockade becomes more important when \( E_c \) increase.

Figure 4 shows the experimental results agree with the theoretical expectations very well, demonstrating good control in the experiments. On the other hand, we can also observe a slight discrepancy between the experimental data and the theoretical ones, which can be attributed to the inhomogeneity of the RF and static fields, the imperfection of the shaped pulses, the inaccuracy of the relaxation parameters and the instability of the sample, etc. We used the same PPS \( \rho_{\text{NMR}} \) for these two cases as the initial ground state because its imperfection only causes the errors of less than 1% on the measurement of \( \langle M_z \rangle \). The main errors come from the imperfection of the quantum adiabatic evolution and the relaxation of the quadrupolar NMR system. The theoretical average fidelity during the adiabatic evolution is about 90%, which will result in a measurement error.
of around 3.7%. The relaxation process will introduce an error of around 2.5%, comparing the effective decoherence time \( T_2^{\text{eff}} = 800\mu s \) during the sequence of phase-incremented pulses.

4. Discussion and conclusion

The Bose–Hubbard system is not only a fundamental model in many-body quantum physics, but also a useful tool for exploring and exploiting quantum coherence. Instead of realizing BHS via ultracold atoms, we have simulated this model using a quadrupolar NMR system and observed the interesting phenomena of the interaction blockade and single-atom quantum tunneling. In the present experiment, we used the spin-3/2 quadrupolar nucleus sodium (\(^{23}\text{Na}\)) to simulate a three-atom system. To our best knowledge, this is the first experimental work of quantum adiabatic control in quadrupolar NMR systems. As we used only an ensemble of single quantum systems in the experiment, there is no quantum entanglement. However, the present experimental results demonstrate that the ensemble of single quantum systems without entanglement can effectively simulate a BHS. This experiment may provide evidence for recent research, that has argued that quantum contextuality is a fundamental source for quantum speed-up over its classical counterparts [53].

Our experiment has demonstrated that the quadrupolar NMR system is a good workbench of quantum simulation on which to study the BHS and other nonlinear quantum systems. Actually, many-body Bose–Hubbard systems cannot be simulated with polynomial effort in the system size \( n \). Yet the current work elucidates the Schwinger representation of angular momenta and demonstrates them in the first NMR experiment showing non-trivial interaction blockades. Further quantum simulation experimental studies can be executed on a quadrupolar NMR system, such as a kicked-top model [54] which is usually viewed as a quantum chaotic system. The quadrupolar NMR system may also be a good candidate for implementing quantum metrology [55–57]. By making use of the nonlinear quadrupolar interaction \( I_z^2 \) and the multi-level characteristics, we can prepare the well-known spin squeezing states [58] and NOON states [59] that are widely used in metrology to achieve a precision that exceeds the classical measurement.

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