

Route toward classical frustration and band flattening via optical lattice distortion

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We propose and experimentally explore a method for realizing frustrated lattice models using a Bose-Einstein condensate held in an optical square lattice. A small lattice distortion opens up an energy gap such that the lowest band splits into two. Along the edge of the first Brillouin zone for both bands, a nearly flat energy-momentum dispersion is realized. For the excited band, a highly degenerate energy minimum arises. By loading ultracold atoms into the excited band, a classically frustrated XY model is formed, describing rotors on a square lattice with competing nearest and next-nearest tunneling couplings. Our experimental optical lattice provides a regime where a fully coherent Bose-Einstein condensate is observed and a regime where frustration is expected. If we adiabatically tune from the condensate regime to the regime of frustration, the momentum spectra show a complete loss of coherence. Upon slowly tuning back to the condensate regime, coherence is largely restored. Good agreement with model calculations is obtained.

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Introduction. Classically frustrated systems are characterized by highly degenerate ground states, which may result in glassy or liquidlike phases with exotic properties [1–3]. While extensively studied during the last decades, defining their properties is extremely challenging due to the complexity of these systems. Using the experimental platform of cold atoms loaded into optical lattices, which has proven useful for controlled simulations of complex systems [4], could open a new chapter for systematic studies of frustration. The simplest example of a frustrated system is that of spins on a triangular lattice with nearest-neighbor antiferromagnetic couplings. Such geometric frustration was recently experimentally explored in a cold atom setting [5] by using spin degrees of freedom and engineered via external periodic driving. Experimental studies of frustrated systems using cold atoms in optical lattices are met with several difficulties. For example, atoms in the lowest Bloch band typically support tunnel couplings with ferromagnetic order without external driving. Focused engineering of band structure degeneracies must go well beyond the tight-binding approximation, so higher-order tunneling terms do not lift these. Furthermore, driving typically leads to heating and loss of coherence. Frustration may also appear on a square lattice due to different mechanisms. In the Villain model [6], three of the tunneling terms are positive,

while the fourth one, closing the loop around a plaquette, is negative. Another possibility arises from the competition between nearest- and next-nearest-neighbor tunneling terms.

For classical rotors $s_i = (\cos \phi_i, \sin \phi_i)$, the frustrated XY model is [7]

$$H_{XY} = J_1 \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) + J_2 \sum_{\langle\langle ij \rangle\rangle} \cos(\phi_i - \phi_j), \quad (1)$$

with positive J_1, J_2 and the sums over nearest- and next-nearest-neighbor coupling terms, respectively. The above model supports “interaction-induced frustration” rather than geometric frustration. Despite four decades of intense research, the physics of the Villain and frustrated XY models is not fully clarified. Both models, sharing the same universal features, support two symmetries: a continuous one corresponding to particle conservation and chiral Ising-like symmetry. Due to the Mermin-Wagner theorem, the former cannot be spontaneously broken but manifests as a Kosterlitz-Thouless transition. It is believed, but still debated [8–14], that upon lowering the temperature, the models pass through two nearby transitions. The phase emerging between the transitions is argued to be a chiral spin liquid [15]. At zero temperature and the frustration point, $J_1 = 2J_2$, the ground state is a liquid phase. The liquid phase may also survive beyond the frustration point [16], even though a thorough analysis, based on a large N expansion, concluded that it exists only at the frustration point [17]. Spin-wave theory suggests that for $J_2 > 2J_1$ antiferromagnetic order is established in the two sublattices with a relative “collinear” order [7], as a result of the order-by-disorder phenomenon [18]. These speculations await any experimental verification.

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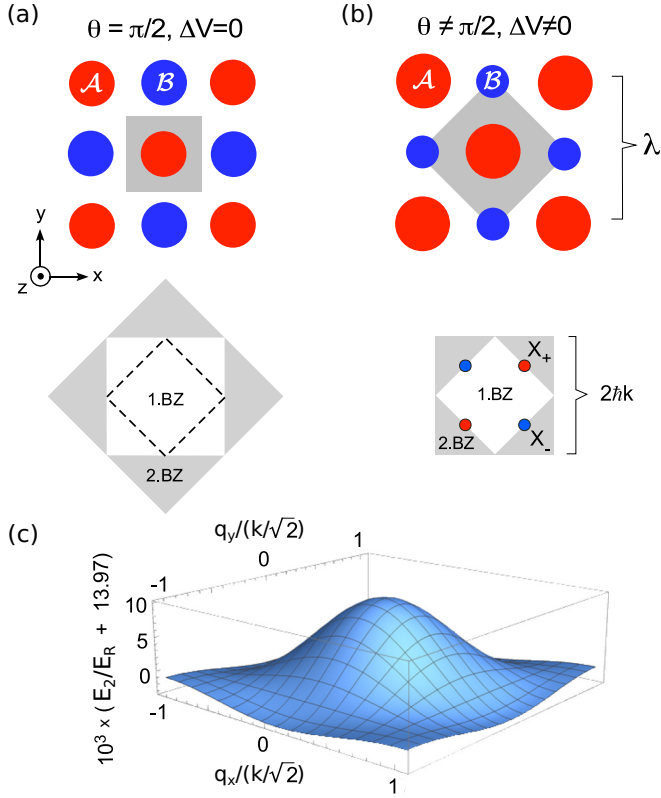


FIG. 1. (a) Conventional square lattice geometry with equivalent $\mathcal{A}$ and $\mathcal{B}$ sites, obtained for $\Delta V = 0$ in Eq. (2). The lower panel shows the first (white square) and second (gray triangles) BZs (the dashed square denotes the reduced BZ for the distorted lattice). (b) Bipartite lattice geometry was obtained for $\Delta V \neq 0$ in Eq. (2) with the corresponding first (white square) and second (gray triangles) BZs in the lower panel. The two inequivalent high-symmetry points $X_{\pm}$ are the global minima of the second band. (c) The second band for $\Delta V \approx 0.063V_0$ and $V_0 = 10E_R$ is plotted across the first BZ.

In this Letter, we propose and experimentally realize a surprisingly simple realization of the frustrated XY model (1) in terms of cold atoms loaded into an optical lattice. The advantage of our method is that no external driving (such as lattice shaking or laser-induced tunneling) is required, which reduces the amount of heating. This realization becomes possible by considering metastable states in higher Bloch bands. In particular, we consider bosonic atoms loaded into the second band of a bipartite square lattice as described in Ref. [19]. This lattice provides two classes of alternating potential wells, denoted $\mathcal{A}$ and $\mathcal{B}$, with tunable relative depths ΔV . In the case $\Delta V = 0$, a simple square lattice arises with a white square denoting the first Brillouin zone (BZ) in Fig. 1(a), surrounded by four gray triangles showing the second BZ. The first Bloch band shows constant energy on the dashed rectangle in Fig. 1(a), dividing the BZ into two equally sized areas. Tuning ΔV slightly away from zero has significant consequences. The unit cell area increases by a factor of two, i.e., the size of the first BZ shrinks by a factor of two, such that it is now bordered by the dashed rectangle [Fig. 1(b)]. Hence, the lowest band of the $\Delta V = 0$ lattice splits into two new bands, thus giving rise to the first and second bands of the $\Delta V \neq 0$ lattice. If ΔV is

kept close to zero, each of these bands is nearly degenerate along the first BZ edge. Thus, the second band provides an extended approximate minimum all along the edge of the first BZ, just as for the frustrated XY model [Fig. 1(c)]. At this stage, our experiment cannot directly confirm the frustration emerging from such a quasidegeneracy. Nevertheless, we show that numerical simulations of the atomic momentum distributions in the frustrated XY model agree well with experimental time-of-flight measurements.

Model system. We consider bosonic atoms within a two-dimensional bipartite optical lattice. Along the transverse third direction, the atoms are confined by a harmonic trap. The two-dimensional lattice is formed by superimposing two one-dimensional standing waves oscillating with a tunable relative phase θ . The optical potential reads

$$V(x, y) = -V_0[\cos^2(kx) + \cos^2(ky)] + 2\cos(\theta)\cos(kx)\cos(ky). \quad (2)$$

In the remainder of this Letter, energies are given in terms of the recoil energy $E_R \equiv \hbar^2 k^2 / 2m$, with k the wave number and m the atomic mass. For $\theta = \pi/2$, a conventional separable square lattice arises [cf. Fig. 1(a)]. When $\theta \neq \pi/2$ [cf. Fig. 1(b)], the last term in Eq. (2) distorts the lattice. This choice of θ gives rise to a bipartite nonseparable lattice geometry composed of two sublattices, with deep and shallow sites $\mathcal{A}$ and $\mathcal{B}$, respectively. Their potential energy difference is $\Delta V = -4V_0 \cos(\theta)$. Due to this distortion, the first BZ is decreased by a factor of two, and the first Bloch band of the $\theta = \pi/2$ lattice splits into two new bands defining a new BZ. These bands are separated by a gap, which for weak distortions scales as $\sim \Delta V / V_0$ according to the “nearly-free-electron gas” model [20]. It is striking how flat the bands are along the BZ edge compared to the band gap. Reaching the regime of frustration requires a flatness characterized by an energy spread that is below the energy associated with the two-body contact interaction between the atoms. Increasing the flatness, however, comes with the price that the bandwidth and the band gap are decreased. Decreasing the bandwidth slows down the relaxation toward the regime of frustration while decreasing the band gap increases the interband relaxation, i.e., the loss of atoms from the second band via collisions [21]. Thus, there is a trade-off in choosing the optimal configuration. For the rest of this Letter, we pick parameters $V_0 = 10E_R$ and $\Delta V = 0.063V_0$, for which we plot the second band in Fig. 1(c). The flatness is not perfect; the bandwidth is about six times the energy spread along the BZ edge, while the gap is roughly 230 times this spread.

To explore the properties of atoms residing solely in the second band, we evoke a single-band approximation and derive an effective lattice model,

$$\hat{H}_1 = \sum_{i \neq j} (t_{ij} \hat{a}_i^\dagger \hat{a}_j + \text{H.c.}), \quad (3)$$

where the matrix t_{ij} amounts to the tunneling amplitudes between sites i and j . These amplitudes can be chosen as real. The above lattice Hamiltonian becomes diagonal by Fourier-transforming it. Using this, we can identify t_{ij} as the Fourier coefficients of the dispersion $E_2(q_x, q_y)$ for the second band of the full Hamiltonian. The relevant numerically extracted

TABLE I. Tunnel matrix for the parameters $V_0 = 10E_R$ and $\Delta V = 0.063V_0$. The first diagonal term gives the on-site energy, the terms (0,1) and (1,0) are the nearest-neighbor tunneling rates J_1 , and (1,1) the next-nearest-neighbor tunneling rate J_2 and so on. All quantities are given in terms of recoil energies E_R .

t_{nm}	0	1	2
0	-13.97	1.4×10^{-3}	-6×10^{-6}
1	1.4×10^{-3}	9.7×10^{-4}	-4×10^{-6}
2	-6×10^{-6}	-4×10^{-6}	-6×10^{-7}

amplitudes are listed in Table I. For the present parameters, it is found that the system is close to the frustrated scenario, i.e., after identifying J_1 and J_2 , we have $J_1/J_2 = 1.43$ while other tunneling terms are approximately zero in comparison. The ratio J_1/J_2 does not equal the desired value 2, implying that the second band is not fully flat along the BZ edge, as seen in Fig. 1(c). The final step in mapping onto the frustrated XY model is accomplished by considering the mean-field approximation. Here, the atomic operators are replaced by their expectations, e.g., $\hat{a} \rightarrow \alpha_i = \sqrt{n_i}e^{i\phi_i}$, such that n_i is the (average) number of atoms at site $\mathbf{i}$ and ϕ_i is the intrasite condensate phase.

We must add one term accounting for the atom-atom interaction and another corresponding to the confining harmonic trap. Following the standard assumptions, i.e., the local density approximation and on-site s -wave scattering, we then derive the mean-field Hamiltonian

$$H = H_1 + \sum_{\mathbf{i}} \frac{\omega^2}{2} n_i |\mathbf{i}|^2 + \frac{U}{2} \sum_{\mathbf{i}} n_i^2, \quad (4)$$

where ω and U are the dimensionless trap frequency and interaction strength, respectively. We can simulate the atomic relaxation that occurs in the experiment (see below) by initializing a state $\psi(\mathbf{i}, 0)$, defined by some set of random variables n_i and ϕ_i , and then evolving this state in imaginary time [22]. If the system is not frustrated, the initial lack of long-range order disappears, and a phase locking among the ϕ_i will occur. For example, if the BZ edge is not flat enough (with minima at the $X_{\pm}$ points), the global condensate builds up a striped order characterized by a π -phase difference between either the columns or rows of the lattice. However, if the BZ is approximately flat, such an order will not build up on any experimentally relevant timescale. In Fig. 2, we show properties of the condensate obtained from numerical simulations. Here, at a given time t , the condensate order parameter is obtained from $\Psi(x, y) = \sum_{\mathbf{i}} \alpha_i w_i(x, y)$, where $w_i(x, y)$ is the Wannier function at site $\mathbf{i}$, which for the figure has been taken as a real Gaussian. From $\Psi(x, y)$ we get the atomic real space and momentum densities $\rho(x, y) = |\Psi(x, y)|^2$ and $\tilde{\rho}(p_x, p_y)$, respectively. We note how the relaxation causes the momentum distribution [Fig. 2(c)] to assemble along the BZ edge. The spatial density [Fig. 2(a)] shows an envelope following the inverse shape of the trap with seemingly complex local density fluctuations stemming from the frustration. A manifestation of the frustration is especially evident in Fig. 2(b) where we plot the condensate phase $\phi(x, y) = \text{angle}[\Psi(x, y)]$. If we let the condensate relax further, i.e., by propagating the simulation

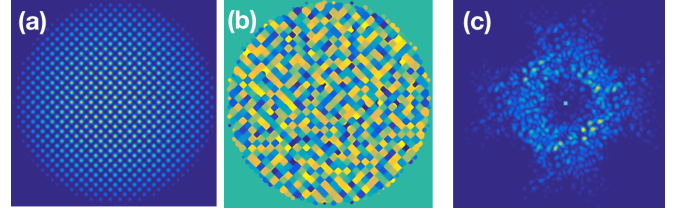


FIG. 2. Numerical simulation of (a) the atomic real-space density, (b) its phase, and (c) the momentum density profile. The relaxation is mimicked by imaginary-time propagation for a dimensionless time $t_f = 100$. At this stage, the condensate is still fairly uniformly distributed around the BZ edge (c). The middle plot (b) shows how no evident order is established in the condensate, which signals the presence of frustration. The system parameters are chosen to represent the experimental ones; the dimensionless trapping frequency $\omega = 0.037$, $V_0 = 10E_R$, $\Delta V = 0.063V_0$, $U_0 = 0.011E_R$, and the number of atoms $N = 10^5$. While the atom-atom interaction manifests in the real-space density profile for these parameters, it has very little influence on the frustration.

further, the momentum distribution would get increasingly concentrated around the $X_{\pm}$ points, and domains of striped order would form in the spatial condensate density. This is demonstrated in Fig. 3 with three different snapshots of the condensate phase. While the growth of the domain sizes slows down, eventually full long-range order should be established. In order to quantify the localization of the momentum distributions in momentum space we also show the second Rényi entropy $R_2(t) = -\log[\frac{\int \tilde{\rho}^2(p_x, p_y) dp_x dp_y}{\int \tilde{\rho}(p_x, p_y) dp_x dp_y}]$ in the figure, where we have used the natural logarithm. The decrease of $R_2(t)$ signals localization, and we have verified that this effect is stronger than if we would be at the exact frustration point for which the whole BZ edge becomes degenerate and not only the $X_{\pm}$ points.

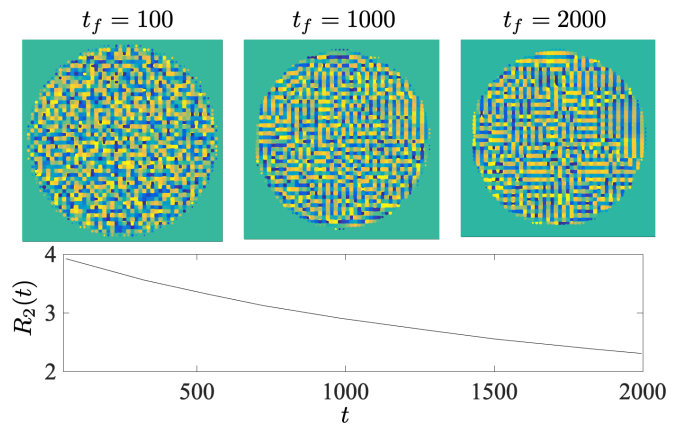


FIG. 3. Snapshots of the condensate phase obtained from the numerically simulated relaxation. The leftmost plot is similar to that of Fig. 2(b). The buildup of intersite order becomes clear in the middle plot, and the growth of domains is demonstrated in the right plot. The lower plot displays the Rényi entropy demonstrating the density clustering around the $X_{\pm}$ points in momentum space. The parameters are the same as those used for Fig. 2, but with one-fourth of the trap frequency ω in order to capture more domains.

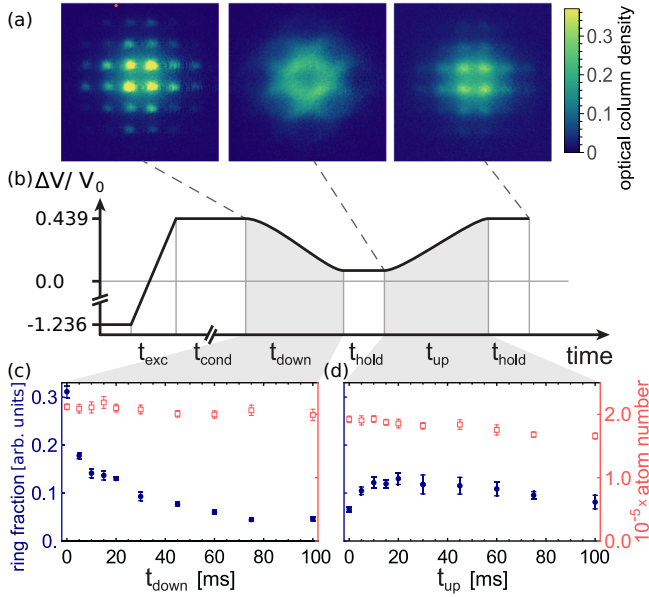


FIG. 4. Collapse and revival of coherence. Three momentum spectra are shown in (a) for characteristic values of ΔV tuned according to the protocol in (b). The first image at $\Delta V = 0.439 V_0$ shows coherent condensate fractions at the $X_{\pm}$ points of the second band [cf. Fig. 1(b)]. In the second image at $\Delta V = 0.063 V_0$ coherence has completely vanished. The third image, recorded after ramping back to $\Delta V = 0.439 V_0$, shows partially restored coherence. The blue disks in (c) and (d) show the observed collapse and revival of coherent condensate fractions at the $X_{\pm}$ points plotted against the ramp times t_{down} and t_{up} , respectively. The red open squares indicate the total population of the first and second bands. Error bars correspond to the standard deviation of the mean for a set of eight measurements.

Experimental demonstration. A nearly pure spin-polarized Bose-Einstein condensate of 3×10^5 rubidium (^{87}Rb) atoms in the hyperfine state $|F = 2, m_F = 2\rangle$ with a temperature of 30 nK is produced in a crossed optical dipole trap (ODT). The atomic sample is adiabatically loaded into a bipartite optical square lattice, which displays a double-well structure as described in Eq. (2). The optical lattice is formed by two mutually orthogonal optical standing waves with a wavelength of $\lambda = 1064$ nm. The lattice depth V_0 and the potential energy difference ΔV can be actively tuned. The tuning of ΔV is realized via the control of the time phase difference θ between the standing waves with a precision of $\pi/300$ conforming to $\Delta V = -4V_0 \cos(\theta)$. A rapid adjustment of ΔV allows us to quench the atoms into higher Bloch bands. For technical details, see Refs. [23,24].

The experimental sequence is performed as follows (cf. Fig. 4): The atoms are initially loaded into the lowest band of the lattice by adiabatically ramping up the lattice depth V_0 to $10E_R$ in 150 ms with fixed $\Delta V = -1.236 V_0$. In addition, we are able to reduce the temperature of the atomic sample by simultaneously decreasing the potential depth of the ODT. After a hold time of 100 ms, a quench protocol is applied to excite the atoms into a metastable second Bloch band [21] by rapidly tuning ΔV to $0.439 V_0$ in $t_{\text{exc}} = 0.1$ ms. After a holding time of $t_{\text{cond}} = 500$ ms, the atoms are condensed at the two inequivalent energy minima of the band, i.e. the $X_{\pm}$ points [cf. Fig. 4(a), left]. Subsequently, the potential difference ΔV

is ramped down during a variable time $t_{\text{down}} \in \{0, 100\}$ ms to $\Delta V = 0.063 V_0$. After $t_{\text{hold}} = 0.02$ ms the potential is ramped back to $\Delta V = 0.439 V_0$ in a variable time $t_{\text{up}} \in \{0, 100\}$ ms for a fixed t_{down} and the atoms are held in the lattice for another $t_{\text{hold}} = 0.02$ ms. Finally, the lattice and trapping potentials are instantaneously switched off, followed by a ballistic expansion of 22 ms and the momentum spectrum is recorded via an absorption image. The temporal evolution of the coherent fraction $(n_{\text{coh}} - n_{\text{incoh}})/(n_{\text{coh}} + n_{\text{incoh}})$ of the population at the $X_{\pm}$ points is observed. This observable is determined by counting the atoms in a disk-shaped region of interest (ROI) around both $X_{\pm}$ points n_{coh} and subtracting the atoms n_{incoh} enclosed by a ring-shaped ROI with the same area of the disk-shaped ROIs [21].

Figure 4(a) shows momentum spectra at $\Delta V = 0.439 V_0$ before the down-ramp (left), at $\Delta V = 0.063 V_0$ after the $t_{\text{down}} = 60$ ms down-ramp and a short hold time $t_{\text{hold}} = 20 \mu\text{s}$ (center), and after the $t_{\text{up}} = 20$ ms up-ramp back to $\Delta V = 0.439 V_0$ followed by $t_{\text{hold}} = 20 \mu\text{s}$ (right). At $\Delta V = 0.439 V_0$, the second band possesses distinct energy minima at the $X_{\pm}$ points, and a coherent condensate fraction is observed as indicated by the visible higher-order Bragg resonances. When the potential difference is ramped down to $\Delta V = 0.063 V_0$ [cf. Fig. 4(b)], the condensate fraction decreases. As illustrated by the blue data points in Fig. 4(c), if the down-ramp time t_{down} is sufficiently large (>60 ms) to satisfy adiabaticity, the condensate fraction practically vanishes, and the atomic sample no longer displays coherence. At $\Delta V = 0.063 V_0$, the energy-momentum dispersion of the second band is almost degenerated along the edge of the first Brillouin zone. The atoms are observed to spread over the entire edge of the second Bloch band populating all available Bloch states. The associated momentum distribution in the center image of Fig. 4(a) shows a rectangular shape, similar to the theoretical prediction of Fig. 2(c). The loss of coherence indicates that the condensate suffers from excessive fragmentation due to the large number of nearly degenerate minimal energy states.

In order to exclude the possibility that the observed vanishing of coherence is due to uncontrolled heating, we have added a second stage in the experimental protocol in Fig. 4(b), where ΔV has ramped up again to the initial value $\Delta V = 0.439 V_0$. If this ramp is processed adiabatically, we observe a revival of the condensate fraction, as is seen in the right-hand image in Fig. 4(a). Figure 4(d) shows that the recovery of the condensed fraction at the $X_{\pm}$ points requires a sufficiently long ramp time t_{up} to satisfy adiabaticity. Maximum coherence is found for t_{up} around 20 ms. The total number of atoms in the first and second band remains nearly constant throughout the measurement [red markers in Fig. 4(c) and 4(d)]. The observed recovery of the condensate fraction appears incomplete, possibly due to residual band relaxation at $\Delta V = 0.063 V_0$ and associated heating processes. These findings indicate that the observed loss of coherence, when tuning to $\Delta V = 0.063 V_0$, could be interpreted as a signature of a glassy phase originating from the massive degeneracy of the second band. A similar protocol was used in Ref. [25] to discriminate a Mott insulation phase from a thermally incoherent phase.

Conclusion. We proposed a method, relying on a lattice distortion, for realizing frustrated models in an optical lat-

tice system. Our proposal does not rely on any driving as in earlier schemes, but the desired antiferromagnetic tunneling terms result naturally by considering the first excited band. The method was experimentally demonstrated by loading a gas of ultracold atoms into this second band. The condensate coherence fraction was measured upon tuning from a nonfrustrated to a frustrated regime and then back. In the frustrated regime, no visible signatures of coherence were observed, in agreement with numerical simulations of the frustrated system, while coherence was partially reestablished after ramping back to the nonfrustrated regime. In a strict sense, this is no direct evidence of frustration, which

would require different experimental tools, e.g., single-site pair-correlation measurements could give more insight into a possible glass and liquid phases. Nevertheless, our work is a step in realizing systematic experimental studies of frustrated matter.

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