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Elastic multibody interactions on a lattice

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We show that by coupling two hyperfine states of an atom in an optical lattice one can independently control two-, three-, and four-body on-site interactions in a nonperturbative manner. In particular, under typical conditions of current experiments, one can have a purely three- or four-body interacting gas of ^{39}K atoms characterized by on-site interaction shifts of several 100 Hz.

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Effective multibody interactions can arise even in a purely two-body interacting system when one integrates out some of its (high-energy) degrees of freedom or substitutes the actual two-body potential by a pseudopotential. Such effective forces are important in many fields from nuclear and high-energy physics to ultracold gases. A textbook example is the appearance of an effective three-body force in the zero-range pseudopotential description of the hard-sphere Bose gas [1,2]. Inclusion of a three-body renormalizing potential (three-body parameter) is unavoidable for a resonantly interacting Bose gas [3]. We can name a few other systems for which multibody interactions are important. The quasi-one-dimensional (1D) Bose gas is kinematically 1D, but virtual transversal excitations lead to the appearance of local three-body terms in the corresponding effective 1D model and break integrability [4–6]. Similar terms enter the single-Landau-level description of quantum Hall systems when one takes into account virtual excitations to other Landau levels [7–9]. Inclusion of these small corrections can lead to qualitative modifications of the phase diagram and can stabilize phases otherwise predicted to be unstable. For bosonic atoms in an optical lattice, effective multibody interactions emerge when one reduces this continuum system to the single-band Hubbard model [10–13]. In spite of their weakness compared to the two-body interaction, they can be measured spectroscopically [14] and give rise to a peculiar collapse and revival dynamics [15–18].

In recent years various possibilities to independently control multibody interactions have been discussed and a number of more or less technically complicated schemes have been suggested [19–29]. The task is not straightforward but highly rewarding because of many potentially interesting implications, in particular, for the creation of topological quantum Hall phases [30], stabilizing paired bosonic superfluids [22,31–34], observing self-trapped droplets [35], and other phenomena [36–43].

A system in which the (effective) three-body interaction is strong and the (effective) two-body one is negligible is unnatural but not impossible. It requires that the two-body scattering amplitude vanish but the wave function nevertheless differ from the truly noninteracting one. This difference can be thought of as a virtually excited two-body state which can scatter other particles. The resulting multibody interactions can thus become strong for sufficiently exotic interaction potentials or single-particle wave functions. In Ref. [29] we have considered the interlayer potential for dipoles in the bilayer geometry and have shown a way to tune it to a two-body zero crossing, at the same time obtaining a strong three-body repulsion.

In this Rapid Communication we extend this idea to a two-component Bose gas in an optical lattice. In this case one can make single-particle wave functions *exotic* by coupling two internal states with a nearly resonant field (the so-called free-free transition [44]). By varying the corresponding Rabi frequency Ω and detuning Δ one can rotate the wave function in the space of the two dressed states and thus tune the two-body interaction, for instance, to a zero crossing. We show that in contrast to what one can obtain near a usual Feshbach zero crossing [45–47], in our case multibody interactions can be made much stronger and elastic. Curiously, the same technique without additional efforts can be used to make the two- and three-body interactions vanish while keeping a finite four-body one. We discuss implications of these results for current experiments and show that favorable conditions (suitable window of inter- and intrastate scattering lengths) are provided by hyperfine states $F = 1, m_F = 0$ and $F = 1, m_F = -1$ of ^{39}K.

Considering the frequency of the hyperfine transition (typically 10^7–10^8 Hz) the largest energy scale in our problem we write the Hamiltonian in the rotating wave approximation as

$$H = \int_{\boldsymbol r}\Big\{\sum_\sigma \Psi^\dagger_{\sigma\boldsymbol r}\big[-\nabla^2_{\boldsymbol r}/2 + V_{\rm ext}(\boldsymbol r)\big]\Psi_{\sigma\boldsymbol r} + \frac{\Delta}{2}(\Psi^\dagger_{\downarrow\boldsymbol r}\Psi_{\downarrow\boldsymbol r} - \Psi^\dagger_{\uparrow\boldsymbol r}\Psi_{\uparrow\boldsymbol r}) - \frac{\Omega}{2}(\Psi^\dagger_{\uparrow\boldsymbol r}\Psi_{\downarrow\boldsymbol r} + \Psi^\dagger_{\downarrow\boldsymbol r}\Psi_{\uparrow\boldsymbol r})\Big\} + \frac{1}{2}\int_{\boldsymbol r,\boldsymbol r'}\sum_{\sigma,\sigma'}\Psi^\dagger_{\sigma\boldsymbol r}\Psi^\dagger_{\sigma'\boldsymbol r'}V_{\sigma\sigma'}(|\boldsymbol r - \boldsymbol r'|)\Psi_{\sigma\boldsymbol r}\Psi_{\sigma'\boldsymbol r'}, \quad (1)$$

where $\Psi^\dagger_{\sigma\boldsymbol r}$ is the creation operator of a boson in the internal (dressed) state $\sigma(=\uparrow,\downarrow)$ with coordinate $\boldsymbol r$, $V_{\rm ext}$ is the external potential of the optical lattice, and $V_{\sigma\sigma'}(r)$ are the short-range interparticle interactions, which are characterized by the s-wave scattering lengths $a_{\sigma\sigma'}$, and we adopt the units $\hbar = m = 1$.

For a single particle, the orbital and spinor degrees of freedom, respectively described by the first and second lines in Eq. (1), decouple. The former is characterized by the usual band structure in the periodic potential $V_{\rm ext}$ and the diagonalization of the latter gives two spinor eigenstates split in energy by $\sqrt{\Omega^2 + \Delta^2}$. We will assume that the temperature of the system is lower than this spinor gap so that the gas is effectively spinless. However, this gap should not be too large in order to allow for virtual excitations of the upper spinor branch during collisions. The lower the gap, the stronger are the multibody interactions.

Let us introduce the *bare* on-site interaction shifts $g_{\sigma\sigma'}$. In the harmonic approximation for the on-site confinement they equal $g_{\sigma\sigma'} = \sqrt{2/\pi}a_{\sigma\sigma'}/l_x l_y l_z$, where l_x, l_y, and l_z are the oscillator lengths. We assume that Ω and $g_{\sigma\sigma'}$ are (i) much smaller than the on-site confinement frequencies and (ii) much larger than the intersite tunneling amplitude t. Condition (i) allows us to use the single orbital mode approximation and completely neglect virtual excitations to higher orbital bands considering the spinor sector as the major source of effective interactions. Assumption (ii) ensures that when a particle tunnels, the wave function has enough time to adjust itself to the ground state for the new configuration of the on-site occupations. It also allows us to neglect the nearest neighbor and more distant effective interactions [48]. Note that the *effective* on-site interaction does not have to be larger than t.

With these assumptions we reduce our original problem to the spinless Bose-Hubbard model with the on-site energy term

$$E(N) = -\frac{\sqrt{\Omega^2+\Delta^2}}{2}N + \sum_{i=2}^{N} U_i \frac{N!}{i!(N-i)!}, \qquad (2)$$

which is the ground-state energy of N bosons governed by the Hamiltonian

$$H_0 = \frac{\Delta}{2}(b_\downarrow^\dagger b_\downarrow - b_\uparrow^\dagger b_\uparrow) - \frac{\Omega}{2}(b_\uparrow^\dagger b_\downarrow + b_\downarrow^\dagger b_\uparrow) + \sum_{\sigma,\sigma'} \frac{g_{\sigma\sigma'}}{2} b_\sigma^\dagger b_{\sigma'}^\dagger b_\sigma b_{\sigma'}. \qquad (3)$$

For a given N one can use the set of $N+1$ wave functions $|i,N-i\rangle$ describing the Fock states of i $\uparrow$ bosons and $N-i$ $\downarrow$ ones. The Hamiltonian Eq. (3) in this representation becomes a symmetric tridiagonal matrix with diagonal elements

$$\begin{aligned}\langle i,N-i|H_0|i,N-i\rangle &= \Delta(N-2i)/2 + g_{\uparrow\uparrow}i(i-1)/2 + g_{\uparrow\downarrow}i(N-i) \\ &\quad + g_{\downarrow\downarrow}(N-i)(N-i-1)/2\end{aligned} \qquad (4)$$

and off-diagonal ones

$$\langle i,N-i|H_0|i+1,N-i-1\rangle = -\frac{\Omega\sqrt{(N-i)(i+1)}}{2}. \qquad (5)$$

Its diagonalization is straightforward and Eq. (2) can be applied iteratively to find U_N, given the knowledge of U_M for all $M<N$.

The five-dimensional parameter space $\{\Omega,\Delta,g_{\sigma\sigma'}\}$ provides enough freedom for an independent control over U_N, at least for several lowest N. When Δ, Ω, and $g_{\sigma\sigma'}$ are of the same order of magnitude, the problem is nonperturbative, the multibody interaction constants U_N are comparable to each other (cf. Refs. [11,18]), and quite exotic combinations of them are possible. However, let us limit our discussion to the most radical *N-body interacting* case, in which finite U_N comes along with vanishing (or very small) U_M for all $M<N$. First we discuss the three-body interacting case, taking into account, as much as possible, current experimental constraints. This sets the following optimization problem. For a given combination of $g_{\sigma\sigma'}$, maximize $U_3>0$ with respect to Ω and Δ with the constraint $U_2=0$.

Most clearly the mechanism behind the effective three-body interaction can be seen for $\Omega=\Delta=g_{\uparrow\downarrow}=0$ and $g_{\downarrow\downarrow}=g_{\uparrow\uparrow}=g>0$. In this case the two-body ground state is $|1,1\rangle$, leading to $U_2=0$. The ground state for $N=3$ is doubly degenerate, spanned by $|2,1\rangle$ and $|1,2\rangle$. The effective three-body interaction equals $U_3=g$ and is generated by the spinor frustration: Each pair prefers to be in the $\uparrow\downarrow$ singlet state—the condition, which cannot be simultaneously satisfied for all $N>2$ particles. It is thus crucial that there are only two internal states. Vanishing Ω is not consistent with some of our initial assumptions, but it is clear that the result does not change much if $t,T \ll \Omega \ll g$, and we still arrive at $U_3 \approx g$.

In the case of generally different $g_{\sigma\sigma'}$ the solution of our optimization problem is $\Omega=0$, $\Delta=g_{\uparrow\downarrow}\,\mathrm{sgn}(g_{\downarrow\downarrow}-g_{\uparrow\uparrow})$, the maximum equals

$$U_{3,\max} = \begin{cases}\min(g_{\downarrow\downarrow},g_{\uparrow\uparrow}), & |g_{\downarrow\downarrow}-g_{\uparrow\uparrow}| > -g_{\uparrow\downarrow}, \\ \max(g_{\downarrow\downarrow},g_{\uparrow\uparrow}) + g_{\uparrow\downarrow}, & |g_{\downarrow\downarrow}-g_{\uparrow\uparrow}| < -g_{\uparrow\downarrow},\end{cases} \qquad (6)$$

and the inequalities

$$0 < \min(g_{\downarrow\downarrow},g_{\uparrow\uparrow}), \quad -\max(g_{\downarrow\downarrow},g_{\uparrow\uparrow}) < g_{\uparrow\downarrow} < 0 \qquad (7)$$

define the region that is interesting for us, where $U_2=0$ and $U_3>0$. Indeed, by treating the off-diagonal terms of H_0 perturbatively, one can show that for any given combination of $g_{\sigma\sigma'}$ satisfying Eq. (7), the point $\Omega=0$, $\Delta=g_{\uparrow\downarrow}\,\mathrm{sgn}(g_{\downarrow\downarrow}-g_{\uparrow\uparrow})$ is a (local) maximum of U_3 along the curve $U_2(\Omega,\Delta)=0$. The correction is quadratic in Ω and one can introduce a finite Ω while maintaining U_3 close to this maximum. Note that the three-body interaction obtained in this manner is linear in $g_{\sigma\sigma'}$. This result is to be compared with the dependence $U_3 \propto g^2/\omega$ which arises from virtual excitations to higher *orbital* bands with the interband spacing given by the on-site oscillation frequency ω [11]. In our case the quadratic dependence $U_3 \propto g^2/\Omega$ would arise for $g_{\sigma\sigma'} \ll \Omega$ in the second-order perturbation theory. Thus, the gain in the amplitude of the three-body effective interaction in the spinor case compared to the orbital one is due to a smaller gap ($\Omega \ll \omega$) between the low-energy and high-energy (virtual) degrees of freedom. Accordingly, U_3 is maximized in the most nonperturbative limit $\Omega \to 0$.

We apply the above formalism to the case of ^{39}K in which $a_{\sigma\sigma'}$ for various hyperfine states have been studied theoretically [49,50] and experimentally [49]. In particular, conditions Eq. (7) are satisfied for the second and third lowest hyperfine states, $F=1,m_F=0\,(\sigma=\downarrow)$ and $F=1,m_F=-1\,(\sigma=\uparrow)$, in the magnetic field region from $B=56$ to 59 G. More specifically, in this region $a_{\uparrow\uparrow}$ decreases from approximately 1.85 to 1.56 nm, $a_{\uparrow\downarrow}$ increases from -2.83 to -2.75 nm, and the point $B_0=59.3(6)$ marks a Feshbach resonance in the $\downarrow\downarrow$ channel with the width $\Delta B \approx -10$ G and background scattering length of approximately -0.95 nm.

For concreteness let us choose $a_{\downarrow\downarrow}=9.4$ nm, $a_{\uparrow\uparrow}=1.7$ nm, and $a_{\uparrow\downarrow}=-2.8$ nm, which should be, within the claimed theoretical and experimental error bars, a good estimate of the scattering lengths at about -1 G detuning from the resonance. Then, let us assume an optical lattice with the lattice constant $\lambda/2=532$ nm and intensity $V_0=15E_R$ ($E_R=2\pi^2\hbar^2/m\lambda^2$) in each of the three spatial directions. This produces [51] a three-dimensional lattice with an isotropic on-site confinement of the frequency $\omega \approx 2\pi \times 35$ kHz (oscillator

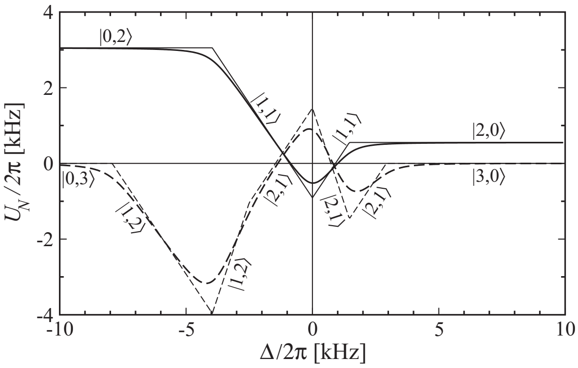

FIG. 1. U_2 (thick solid) and U_3 (thick dashed) vs Δ for $\Omega = 2\pi \times 0.5$ kHz. The thin piecewise linear curves correspond to the limit of vanishing Ω where Fock states $|i,N-i\rangle$ are exact eigenstates (see labels). The point that is interesting for us, where $U_2 = 0$ and $U_3 > 0$, is given by $\Delta = -2\pi \times 0.87$ kHz, $U_3 = 2\pi \times 0.48$ kHz, and can be compared to the case $\Omega = 0$ where $\Delta = g_{\uparrow\downarrow} = -2\pi \times 0.9$ kHz, $U_3 = g_{\uparrow\uparrow} = 2\pi \times 0.55$ kHz.

lengths $l = l_x = l_y = l_z \approx 86$ nm), intersite tunneling amplitude $t \approx 2\pi \times 30$ Hz, and the on-site interaction shifts $g_{\downarrow\downarrow} \approx 2\pi \times 3.05$ kHz, $g_{\uparrow\uparrow} \approx 2\pi \times 0.55$ kHz, and $g_{\uparrow\downarrow} \approx -2\pi \times 0.91$ kHz.

In Fig. 1 we plot U_2 (thick solid line) and U_3 (thick dashed line) versus Δ for $\Omega = 2\pi \times 0.5$ kHz. For comparison we also show the case $\Omega \to 0$ where the ground states are Fock states and $U_2(\Delta)$ and $U_3(\Delta)$ become piecewise linear functions. Each segment of them is labeled accordingly and the corresponding values of $E(N)$ and U_N can be restored from Eqs. (2) and (4). For small finite Ω the segment junctions smoothen and follow the lower or upper branches of three-body, two-body, or one-body (for $\Delta = 0$) level anticrossings. In the example shown of $\Omega = 2\pi \times 0.5$ kHz there are two zero crossings of U_2. The right one corresponds to negative U_3, but at the left crossing point we obtain $U_3 = 2\pi \times 0.48$ kHz, to be compared with $U_{3,\max} = g_{\uparrow\uparrow} = 2\pi \times 0.55$ kHz [see Eq. (6)]. We see that a rather strong elastic three-body effective interaction can coexist with the vanishing two-body one.

A possible practical issue related to this proposal is that three atoms on a single site can recombine to a deeply bound molecule. This loss process can be accounted for by a negative imaginary part of U_3, which, for nonresonant two-body interactions, is proportional to $(R_{\mathrm{vdW}}^4/m)\int|\phi_0(\mathbf{r})|^6 d^3r \propto R_{\mathrm{vdW}}^4/ml^6$. Here ϕ_0 is the on-site ground-state wave function and the van der Waals range R_{vdW} is of the same order of magnitude as $a_{\sigma\sigma'}$. Note that $|\mathrm{Im}\,U_3|/\mathrm{Re}\,U_3 \sim (R_{\mathrm{vdW}}/l)^3$ is very small. More quantitatively, by adopting the free-space loss rate formula to the case of a single confined triple we derive $\mathrm{Im}\,U_3 = -(K_3/3!)\int|\phi_0(\mathbf{r})|^6 d^3r$, where K_3 is the three-body recombination loss rate constant for noncondensed atoms. For nonresonant ^{39}K it is rather small [52], $K_3 < 10^{-29}$ cm^6/s. For the considered scattering lengths, to be on the safe side, we assume $K_3 < 10^{-27}$ cm^6/s and arrive at $-\mathrm{Im}\,U_3 < 2\pi \times 0.4$ Hz $\ll \mathrm{Re}\,U_3$.

Another potential problem can be fluctuations δB of the magnetic field causing an instability of the resonant radio frequency $\Delta_0(B)$ for the hyperfine transition, which,

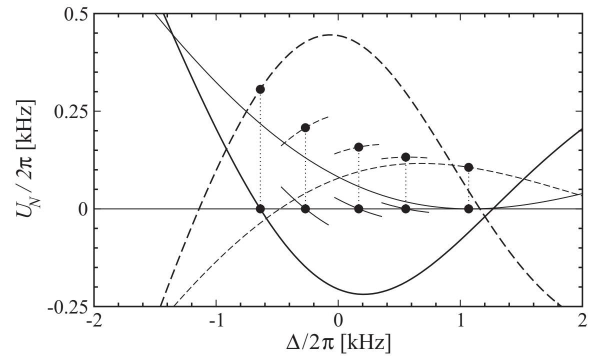

FIG. 2. U_2 (solid) and U_3 (dashed) vs Δ for $\Omega/2\pi = 1.3$, 2.06, 2.69, 3.09, and 3.33 kHz in the vicinities of two-body zero crossings (circles). The whole curves are plotted for the lowest (thick) and highest (thin) values of Ω. At the crossings $-dU_2/d\Delta = 1/2$, 1/4, 1/8, 1/16, and 0, respectively.

in turn, gives rise to fluctuations of the two-body interaction $\delta U_2 = -(dU_2/d\Delta)[d\Delta_0(B)/dB]\delta B$. The first derivative $d\Delta_0(B)/dB$ depends on the atom, hyperfine states, and magnetic field. For the considered hyperfine states of ^{39}K at $B \approx 58$ G it equals $d\Delta_0(B)/dB \approx 2\pi \times 0.7$ kHz/mG [53]. The derivative $dU_2/d\Delta$ for small Ω equals $dU_2/d\Delta \approx -1$. In this case, in order to realize $|U_3| \gg |U_2|$, the magnetic field fluctuations should be kept below 1 mG. However, $dU_2/d\Delta$ decreases with Ω faster than U_3. In Fig. 2 we show $U_2(\Delta)$ and $U_3(\Delta)$ close to two-body zero crossings for Ω chosen such that at the crossings $-dU_2/d\Delta = 1/2, 1/4, 1/8, 1/16$, and 0, respectively. To avoid cluttering we show the whole curves only for the cases $\Omega = 2\pi \times 1.3$ kHz ($dU_2/d\Delta = -1/2$) and $\Omega = 2\pi \times 3.33$ kHz for which $U_2(\Delta)$ touches the horizontal axis ($dU_2/d\Delta = 0$). In the latter case U_3 is just above 100 Hz, but the restriction on the magnetic field stability is relaxed.

Let us now turn to the four-body and higher-order interactions. The N-body interacting case, $U_2 = U_3 = \cdots = U_{N-1} = 0$ and $U_N > 0$, can in principle be realized by extending the spin frustration idea to an atom with $N-1$ internal states, provided repulsive intrastate interactions and attractive interstate ones. Then, $N-1$ atoms on a single site can avoid the intrastate repulsion by occupying different internal states. However, for a larger number of atoms at least two of them have to be in the same state, leading to a positive energy shift.

It turns out that the four-body interacting case can be realized by coupling only two internal states. Indeed, in Fig. 2 we notice that the points $U_2 = U_3$ for $\Omega = 2\pi \times 1.3$ kHz and for $\Omega = 2\pi \times 3.3$ kHz are on different sides of the horizontal axis. We find that $U_2 = U_3 = 0$ for $\Omega = 2\pi \times 1.7$ kHz, $\Delta = 2\pi \times 1.38$ kHz. At this point the four-body interaction is repulsive and equals $U_4 = 2\pi \times 0.18$ kHz (see Fig. 3). We have checked that U_4 can be increased (keeping $U_2 = U_3 = 0$) by decreasing the magnetic field detuning from the $\downarrow\downarrow$ Feshbach resonance (at -0.5 G detuning we obtain $U_4 \approx 0.33$ kHz). However, close to the resonance $a_{\downarrow\downarrow}$ becomes comparable to the oscillator length of the on-site confinement and we can no longer rely on the single-mode approximation. We also expect $\mathrm{Im}\,U_3$ to increase. Nevertheless,

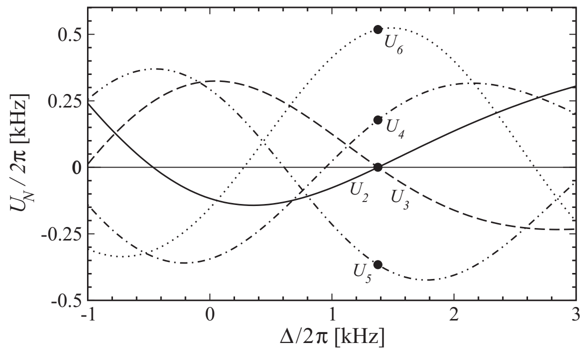

FIG. 3. U_2 (solid), U_3 (dashed), U_4 (dashed-dotted), U_5 (dashed-double dotted), and U_6 (dotted) vs Δ for $\Omega/2\pi = 1.7$ kHz. The circles indicate the corresponding values at the simultaneous two- and three-body zero crossing.

our findings indicate that the four-body interacting case, which seems to be too exotic, is reachable in current experiments.

In Fig. 3 we also show U_5 and U_6 for reference. That U_N changes sign and grows with N is a manifestation of the nonperturbative nature of the problem and can be considered as an artifact of expressing the observable $E(N)$ in terms of U_i's which enter Eq. (2) with numerically large coefficients. The largest contribution to $E(N)$ does not necessarily come from U_N. In particular, at the crossing in the conditions of Fig. 3, U_5 is negative and equals $-2\pi \times 0.366$ kHz, which is twice as large as U_4. Yet, the on-site interaction energy of five atoms equals $5U_4 + U_5 > 0$.

Finally, let us discuss possible experimental signatures of the few-body interactions. The powerful method of Ref. [18] is capable of accurately resolving even very weak multibody interactions. However, our interactions are nonperturbative and we expect much stronger effects and qualitative changes of the many-body phase diagram. For example, a superfluid with $U_2 < 0$ and $U_3 > 0$ (both weaker or comparable to t) should be in the droplet state [35]. In the absence of external trapping (the optical lattice is kept) it would exhibit a solitonlike self-trapping with a flat density $n = -3U_2/2U_3$. Then, increasing both U_2 and U_3 should eventually lead to the paired state [22,41–43]. Another manifestation of multibody interactions is the modification of the Mott-superfluid lobes [38]. In particular, sufficiently deeply in the Mott-insulating state with $n = 2$ atoms per site the excitation gap equals $E(3) + E(1) - 2E(2) = U_3 + U_2$. From Fig. 1 we see that this gap decreases and eventually vanishes as we go from large negative Δ to the point $\Delta \approx -2\pi \times 5$ kHz, which should be detectable by standard methods [51,54]. Note that the insulating state with $n = 1$ does not feel U_3 and thus stays incompressible.

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