Hubbard model for ultracold bosonic atoms interacting via zero-point-energy–induced three-body interactions

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We show that, for ultracold neutral bosonic atoms held in a three-dimensional periodic potential or optical lattice, a Hubbard model with dominant, attractive three-body interactions can be generated. In fact, we derive that the effect of pairwise interactions can be made small or zero starting from the realization that collisions occur at the zero-point energy of an optical lattice site and the strength of the interactions is energy dependent from effective-range contributions. We determine the strength of the two- and three-body interactions for scattering from van der Waals potentials and near Fano-Feshbach resonances. For van der Waals potentials, which for example describe scattering of alkaline-earth atoms, we find that the pairwise interaction can only be turned off for species with a small negative scattering length, leaving the ^{88}Sr isotope a possible candidate. Interestingly, for collisional magnetic Feshbach resonances this restriction does not apply and there often exist magnetic fields where the two-body interaction is small. We illustrate this result for several known narrow resonances between alkali-metal atoms as well as chromium atoms. Finally, we compare the size of the three-body interaction with hopping rates and describe limits due to three-body recombination.

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I. INTRODUCTION

In 1998 Jaksch *et al.* [1] suggested that laser-cooled atomic samples can be held in optical lattices—periodic potentials created by counterpropagating laser beams. These three-dimensional lattices have spatial periods between 400 and 800 nm and depths V_0 as high as $V_0/h \sim 1$ MHz, where h is Planck's constant. An ensemble of atoms then realize either the fermionic or bosonic Hubbard model, where atoms hop from site to site and interact only when on the same site. The interaction-driven quantum phase transition of this model was first realized in Ref. [2].

Today, optical lattices are seen as a natural choice in which to simulate other many-body Hamiltonians. These include Hamiltonians with complex band structure such as double-well lattices [3–6], two-dimensional hexagonal lattices [6–9], as well as those with spin-momentum couplings possibly leading to topological matter [10,11]. Quantum phase transitions in these Hamiltonians enable ground-state wave functions with unusual order parameters, such as pair superfluids and striped phases [12–14]. Phase transitions in Hamiltonians with long-range dipole-dipole interactions using atoms or molecules with large magnetic or electric dipole moments can also be studied. Finally, atoms in optical lattices can be used to measure gravitational acceleration (g) [15–17] and to shed light on nonlinear measurements [18–21] and can be used for quantum information processing.

Over the past ten years ultracold-atom experiments have also investigated few-body phenomena. In particular, three-body interactions have been studied through Efimov physics of strongly interacting atoms observed as resonances in three-body recombination, where three colliding atoms create a dimer and a free atom [22–24]. Here, recent developments include the prediction of a minimum in the recombination rate coefficient K_3 for scattering of a van der Waals potential with a d-wave shape resonance [25]. Moreover, Ref. [26] presented advanced numerical simulations that can quantitatively model observed recombination rates, while Ref. [27] showed empirically that, for a broad ^{7}Li Feshbach resonance, K_3 is controlled by the effective range correction of the atom-atom scattering.

Proposals that suggest ways to create atomic gases dominated by elastic three-body interactions have also been made. In Refs. [28,29] this was achieved by adding resonant radiation to couple internal states of an atom or by driving the lattice at rf frequencies. Some of us showed that the low-energy behavior of atoms in complex lattice geometries (i.e., double-well optical lattices) can also be engineered to lead to large three-body interactions [30]. Interestingly, after the observation of the formation of droplets [31] in a ferromagnetic atomic dysprosium condensate induced by a rapid quench to attractive pairwise interactions, Refs. [32,33] independently suggested that the origin of this instability is large repulsive elastic three-body collisions.

In this paper we propose a way to create dominant three-body interactions in Hubbard models. We rely on two ingredients. The first relies on the analytical analysis of scattering from a van der Waals potential [34,35] as well as analytical modeling of Fano-Feshbach resonances, where the energy of molecular states is tuned with a magnetic field [36].

This analysis confirms that ultracold scattering is describable in terms of a scattering length a and effective range r_e that are uniquely specified by the van der Waals coefficient and resonance parameters. The second ingredient is the realization that two-, three-, and higher-body interaction energies of atoms in an optical lattice site can under certain assumptions be computed analytically [37,38].

We show that for two atoms in a lattice site, with a non-negligible zero-point energy, a cancellation of the contribution from the scattering length and effective range contribution can occur while simultaneously three atoms have a finite inseparable three-body interaction that is of sufficient magnitude that an experimental observation is possible.

This paper is organized as follows. In Sec. II we introduce δ-function interactions between atoms with strength defined by the scattering length and effective range and review results for the ground-state energy of a few atoms held in a site of an optical lattice. We also examine the quality of a harmonic approximation of the lattice site potential. In Sec. III we derive the relationship between a and r_e for which the two-body interactions cancel and three-body interactions remain. Sections IV and V describe how this relationship can be met for a van der Waals potential and for Feshbach resonances, respectively. For scattering from a van der Waals potential we show that the ^{88}Sr isotope is a promising candidate. For Feshbach resonances we work out four cases, one each for ^{23}Na, ^{39}K, ^{52}Cr, and ^{133}Cs scattering. We also compare the expected three-body interaction energies with tunneling energies between lattice sites. Section VI describes two methods to determine lattice parameters for which there are no on-site two-body interactions and discusses limits set by three-body recombination.

II. PSEUDOPOTENTIAL FOR LOW-ENERGY COLLISIONS, OPTICAL LATTICES, AND EFFECTIVE FIELD THEORY

In 1957 Huang [39] showed that the low-energy scattering of two neutral atoms of mass m with an isotropic interatomic potential can be modeled by the equivalent three-dimensional δ-function pseudopotential

$$V_{\rm pseudo}(\vec{R}) = 4\pi\frac{\hbar^2}{2\mu}\left(a - \frac{1}{2}r_e a^2\nabla^2\right)\delta(\vec{R})\frac{\partial}{\partial R}R, \qquad (1)$$

where $\vec{R}$ describes the separation and orientation of the atom pair, ∇ is the gradient operator for the relative motion, $\mu = m/2$ is the reduced mass, and $\hbar = h/(2\pi)$. The scattering length a and the effective range r_e parametrize the effect of the physical interaction potential. (This derivation was revisited in Refs. [40–42].) Crucial for this paper is that a and r_e have a simple relationship and can be tuned near Feshbach resonances.

Our atoms are held in a three-dimensional periodic potential created by counterpropagating laser beams with wave vectors k_L. For simplicity we assume a cubic lattice with potential $V(\vec{x}) = V_0\sum_i \cos^2(k_L x_i)$, where $\vec{x} = (x_1,x_2,x_3)$ is the atomic location and V_0 is the lattice depth. The potential has periodicity π/k_L and a minimum in each unit cell with harmonic

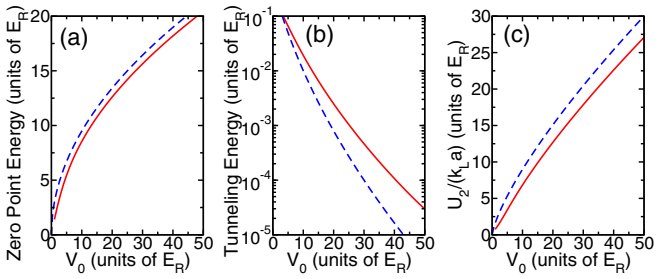

FIG. 1. (a) Zero-point energy, (b) tunneling energies, and (c) the scaled first-order two-body interaction strength $U_2/(k_L a)$ with no effective-range correction as a function of lattice depth V_0 for a cubic, three-dimensional optical lattice. Solid red curves are based on exact band-structure calculations and exact Wannier functions. Dashed blue lines are based on oscillator solutions of the isotropic harmonic approximation around the lattice minima [43].

frequency and single-atom oscillator length given by

$$\hbar\omega = 2\sqrt{V_0 E_R} \text{ and } \ell = \sqrt{\hbar/(m\omega)} = 1/(k_L\sqrt[4]{V_0/E_R}),$$

respectively. Here $E_R = \hbar^2 k_L^2/(2m)$ is the recoil energy.

We rely on this harmonic approximation near the lattice minima. Figures 1(a) and 1(b) show that for sufficiently large V_0 this is qualitatively correct. Figure 1(a) compares the zero-point energy of the harmonic approximation, $3\hbar\omega/2$, with that of the on-site energy of the lowest band obtained from our exact band-structure calculation. The exact on-site energy is always smaller since anharmonic corrections are attractive. Similarly, Fig. 1(b) shows a comparison of the tunneling energies between nearest-neighbor unit cells. Here, the perturbative (harmonic) result underestimates the tunneling energy because anharmonic corrections delocalize the Wannier functions.

The harmonic approximation also simplifies the calculation of the interaction energies between atoms. Nonperturbative eigenenergies for two atoms interacting via a δ-function potential were derived in Ref. [44]. Moreover, Refs. [37,38] perturbatively calculated the ground-state energy $E_{n=2,3,\ldots}$ of two, three, or more atoms based on effective-field theory [45]. In fact, up to second-order perturbation theory when $a \ll \ell$ and $r_e a^2/2 \ll \ell^3$ they showed $E_n = 3n\hbar\omega/2 + U_2 n(n-1)/2 + U_3 n(n-1)(n-2)/6$, where U_2 and U_3 are the two- and three-body interaction strengths

$$U_2/\hbar\omega = \xi + \frac{3}{2}\epsilon + (1-\ln 2)\xi^2 + 2\left(2 - \frac{3}{2}\ln 2\right)\xi\epsilon + \left(\frac{15}{4} - \frac{9}{4}\ln 2\right)\epsilon^2, \qquad (2)$$

and

$$U_3/\hbar\omega = \left\{6 - 4\sqrt{3} - 6\ln\left(\frac{4}{2+\sqrt{3}}\right)\right\}\xi^2 + \left\{24 - \frac{52}{3}\sqrt{3} - 18\ln\left(\frac{4}{2+\sqrt{3}}\right)\right\}\xi\epsilon + \left\{\frac{45}{2} - \frac{55}{3}\sqrt{3} - \frac{27}{2}\ln\left(\frac{4}{2+\sqrt{3}}\right)\right\}\epsilon^2, \qquad (3)$$

with dimensionless quantities

$$\xi = \sqrt{\frac{2}{\pi}}\frac{a}{\ell} \quad \text{and} \quad \epsilon = \sqrt{\frac{2}{\pi}}\frac{1}{2}\frac{r_e a^2}{\ell^3},$$

and $\ln z$ is the natural logarithm. Four- and higher-body interaction strengths are zero at this order of field theory. Reference [46] performed similar calculations for a box with periodic boundary conditions. We ignore small corrections from nonzero partial wave and anisotropic magnetic dipole-dipole scattering.

For completeness Fig. 1(c) compares the two-body interaction strength in a harmonic trap evaluated to first order in a and $r_e = 0$ [i.e., $U_2 = \sqrt{2/\pi}(a/\ell)\hbar\omega$] with the corresponding matrix element based on the energetically lowest Wannier function of the three-dimensional optical lattice. The curves are in sufficiently good agreement such that a harmonic approximation with its analytical results up to second-order perturbation theory can be confidently used for the analysis of U_2 and U_3.

III. CANCELLATION OF THE TWO-BODY INTERACTION

We can now search for parameter regimes where U_2 is small compared to U_3 and, in particular, look for the case $U_2 = 0$. In fact, by factorizing U_2 and requiring that $\xi \ll 1$ and $\epsilon \ll 1$ we realize that if we can achieve

$$\epsilon = -\tfrac{2}{3}\xi \quad \text{or} \quad \tfrac{1}{2}r_e a^2 = -\tfrac{2}{3}a\ell^2 \tag{4}$$

the two-body interaction strength U_2 vanishes as the contributions from the scattering length and the effective range cancel. Equation (4) can be shown to hold to all orders in a and r_e from Ref. [44] [by making the replacement $a \to a + r_e a^2(2\mu E/\hbar^2)/2$ in Eq. (16) of that article]. More importantly, the three-body interaction strength does not vanish and is

$$U_3/\hbar\omega = -\frac{16}{9}\frac{1}{\sqrt{3}}\xi^2 = -\frac{32}{9\pi\sqrt{3}}\frac{a^2}{\ell^2}, \tag{5}$$

which is always attractive and remains of the same order of magnitude as in Eq. (3). The next two sections describe ways in which we can achieve this cancellation.

IV. van der Waals POTENTIAL

Ultracold scattering between structureless ground-state atoms, such as the alkaline-earth atoms, or between more-complex atoms away from any scattering resonance, such as alkali-metal atoms in an external magnetic field, is controlled by its long-range isotropic $-C_6/R^6$ potential, where C_6 is the van der Waals coefficient. This follows from the fact that for separations where deviations from this van der Waals potential due to electron bonding are significant, its depth is already orders of magnitude larger than the initial kinetic energy of the atoms [34,36]. References [47,48] then showed that when the potential has a scattering length a its effective range is

$$\frac{1}{2}r_e a^2 = \frac{1}{3c_e^2}\bar{a}[(a-\bar{a})^2 + \bar{a}^2], \tag{6}$$

where $\bar{a} = c_e(2\mu C_6/\hbar^2)^{1/4}$ is the mean scattering length [35] and $c_e = 2\pi/[\Gamma(1/4)]^2 = 0.4780\ldots$, and $\Gamma(z)$ is the gamma function. For typical atoms $\bar{a}$ lies between $30a_0$ and $100a_0$, where $a_0 = 0.0529$ nm is the Bohr radius. Figure 2 shows the effective range volume $r_e a^2/2$ as a function of a. It is always positive, has a minimum at $a = \bar{a}$, and for $a \to 0$ equals $r_e a^2/2 = 2.918\ldots\bar{a}^3$, which implies that r_e diverges for a zero scattering length.

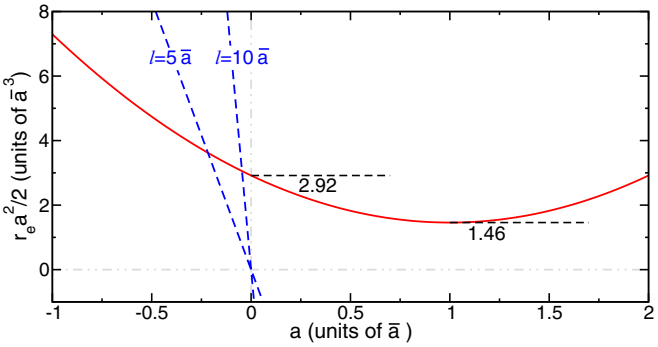

FIG. 2. The effective range volume $r_e a^2/2$ (solid red curve) as a function of scattering length a for a van der Waals potential. All lengths are expressed in units of the mean scattering length $\bar{a}$. The dashed blue curves correspond to $-2a\ell^2/3$ for two values of ℓ. At intersections of $r_e a^2/2$ and $-2a\ell^2/3$ the effective two-body interaction is tuned to zero.

In order to find regimes where U_2 is small compared to U_3, we investigate whether Eq. (4) can hold. This equality is graphically solved in Fig. 2 for two ratios $\ell/\bar{a} \gg 1$, corresponding to typical circumstances in current experiments. We immediately observe that solutions exist for negative scattering lengths that are small compared to $\bar{a}$. In fact, a Taylor expansion for large $\ell/\bar{a}$ gives

$$\frac{a}{\bar{a}} = -\frac{1}{c_e^2}\left(\frac{\bar{a}}{\ell}\right)^2 + O(1/\ell^4) \tag{7}$$

and thus $|a/\bar{a}| \ll 1$ and $|a/\ell| \ll 1$, consistent with our assumptions.

For a van der Waals potential a is fixed. Hence, Eq. (7) is a constraint on ℓ or the trapping frequency ω (and thus on the lattice depth V_0). Moreover, there exist only a few atomic species with the small negative scattering length needed to have a small or vanishing U_2. In fact, we are only aware of the strontium isotope ^{88}Sr to satisfy $|a/\bar{a}| \ll 1$, since it has a scattering length of $a = -2.0(3)a_0$ and $\bar{a} = 71.76a_0$ [49]. (Numbers in parentheses are one-standard-deviation uncertainties.) Hence, we find that $U_2 = 0$ requires $\ell = 900a_0$ and thus $\omega/(2\pi) = 50$ kHz. Assuming a realistic Sr optical lattice with a photon recoil energy of $E_R/h = 4.0$ kHz, we read from Fig. 1(a) that $V_0 \approx 40E_R$ and that from Fig. 1(b) the tunneling energy $J \approx 10^{-4}E_R$ or $J/h \approx 0.4$ Hz. This tunneling energy is comparable to the three-body strength $U_3/h \approx -0.15$ Hz calculated from Eq. (5).

V. FESHBACH RESONANCES

Ultracold scattering of alkali-metal atoms [36] in a magnetic field B contains collisional resonances, where the scattering length can be tuned. Recently, interest has also focused on resonances with atoms with large magnetic moments, such

as Cr [50], Er [51], and Dy [52,53], as the long-range magnetic dipole-dipole interaction influences their collective behavior.

At ultracold collision energies $E = \hbar^2 k^2/(2\mu)$ resonant scattering is described by the scattering amplitude [54–56]

$$f(k) = f_{\rm bg}(k) - e^{2i\delta_{\rm bg}(k)} \frac{\Gamma(E)/2}{E - E_{\rm res}(B,E) + i\Gamma(E)/2}, \quad (8)$$

where $f_{\rm bg}(k) = e^{i\delta_{\rm bg}(k)}\{\sin\delta_{\rm bg}(k)\}/k$ is the background scattering amplitude away from the resonance and $\delta_{\rm bg}(k)$ is the background phase shift. We assume that the low-energy behavior of $f_{\rm bg}(k)$ is that of a van der Waals potential with scattering length $a_{\rm bg}$ as discussed in Sec. IV. The dispersive second term of Eq. (8) describes the resonance with a magnetic-field- and energy-dependent resonance location $E_{\rm res}(B,E) = \mu_e(B - B_0) + \beta E$ and positive energy width $\Gamma(E) = 2(ka_{\rm bg})\Gamma_0(1 + \alpha E/\Gamma_0)$, where μ_e is the magnetic moment of the resonant state, B_0 is the magnetic field at resonance, and Γ_0 is the resonance strength. Finally, the field-independent coefficients α and β describe additional energy dependencies of $\Gamma(E)$ and $E_{\rm res}(E)$ and will affect the effective range.

We note that by definition $\mathrm{Re}\, f(k) = -a - \{r_e a^2/2 - a^3\}k^2 + \cdots$ and a Taylor expansion of Eq. (8) in k then leads to the scattering length $a = a_{\rm bg} - a_{\rm bg}\Gamma_0/E_{\rm res}(B,0)$ and effective range volume

$$\begin{aligned} \tfrac{1}{2}r_e a^2 &= \tfrac{1}{2}r_{\rm bg}a_{\rm bg}^2 + a a_{\rm bg}(a - a_{\rm bg}) - (1-\beta)(a - a_{\rm bg})^2\bar{a}/s_{\rm res} \\ &\quad + \alpha(a - a_{\rm bg})\bar{a}a_{\rm bg}/s_{\rm res} \quad (9) \\ &\equiv V_{\rm q} + g_{\rm q}(a - a_{\rm q})^2, \quad (10) \end{aligned}$$

where $r_{\rm bg}$ is the background effective range given in Eq. (6) when evaluated at scattering length $a_{\rm bg}$. We have eliminated the dependence on $E_{\rm res}(B,0)$ in favor of a and the dimensionless $s_{\rm res} \equiv a_{\rm bg}\Gamma_0/(\bar{a}\bar{E}) > 0$ characterizes the resonance strength in terms of the mean scattering length $\bar{a}$ and energy $\bar{E} = \hbar^2/(2\mu\bar{a}^2)$ of a van der Waals potential [36]. A resonance is narrow when $s_{\rm res} \ll 1$ and broad otherwise. Moreover, the volume $r_e a^2/2 \to r_{\rm bg}a_{\rm bg}^2/2$ when $a \to a_{\rm bg}$ as expected and

$$\tfrac{1}{2}r_e a^2 \to \tfrac{1}{2}r_{\rm bg}a_{\rm bg}^2 - (1 - \beta + \alpha)\bar{a}a_{\rm bg}^2/s_{\rm res}$$

for $a \to 0$, showing that $r_e a^2/2$ can be negative. For narrow resonances this was already noted in Ref. [57].

The effective-range volume near a resonance is a quadratic polynomial in a with coefficients defined by Eq. (10). This dependence agrees with the coupled-channels calculations with rigorous interatomic potentials of Ref. [58]. Their $V_{\rm q}$, $g_{\rm q}$, and $a_{\rm q}$ for a narrow ^{39}K and broad Cs resonance are tabulated in Table I. The corresponding effective-range volume as well as that for a narrow Na resonance based on Eq. (9) with $\alpha = \beta = 0$ are shown in Fig. 3 as a function of a as it is tuned with a magnetic field. For narrow resonances $\alpha,\beta \ll 1$ and α,β have negligible effect on $r_e a^2/2$. For broad resonances with larger α,β their effect is large. For both cases $r_e a^2/2$ is negative and orders of magnitude larger than that for van der Waals potentials.

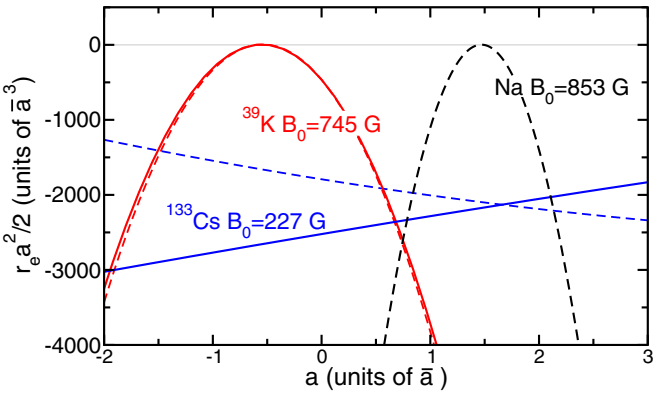

FIG. 3. Effective volume $r_e a^2/2$ of the Feshbach resonances listed in Table I as a function of scattering length a with lengths in units of $\bar{a}$. Solid lines correspond to volumes based on Eq. (9) with $\alpha,\beta \neq 0$ or equivalently the coupled-channels calculation of [58]. Dashed lines follow from Eq. (9) with $\alpha = \beta = 0$.

The model for the effective-range volume now enables us to find scattering lengths where U_2 is small compared to U_3. We set $U_2 = 0$ and Eq. (4) gives

$$V_{\rm q} + g_{\rm q}(a - a_{\rm q})^2 = -\tfrac{2}{3}a\ell^2, \quad (11)$$

where both a and ℓ can be tuned. Coefficients $V_{\rm q}$, $g_{\rm q}$, and $a_{\rm q}$ are fixed by the resonance. Consequently, choosing a fixes the harmonic trapping frequency and vice versa. Crucially and unlike for a van der Waals potential, $r_e a^2/2$ is mostly negative and large compared to $\bar{a}^3$ so that $U_2 = 0$ can occur for positive a on the order of $\bar{a}$. We must, however, also require that $|r_e a^2/2| \ll \ell^3$. This cannot be guaranteed for all resonances. For example, Fig. 3 implies that for the narrow ^{39}K resonance and $a > \bar{a}$ the volume $|r_e a^2/2| \geqslant \ell^3$ assuming typical ℓ between $10\bar{a}$ and $100\bar{a}$. The narrow Na and broader Cs resonances show more promise.

In Fig. 4 we make these observations more precise by plotting U_2 and U_3 as a function of a for four narrow Feshbach

TABLE I. Parameters for five Feshbach resonances. Columns represent the atomic species, B_0 in gauss, the background scattering length $a_{\rm bg}$, resonance strength $s_{\rm res}$, coefficients $V_{\rm q}$, $g_{\rm q}$, and $a_{\rm q}$, where available from Ref. [58], and dimensionless α and β found from a fit to $V_{\rm q}$, $g_{\rm q}$, and $a_{\rm q}$ in Eq. (10). Lengths and volumes are in units of $\bar{a}$ and $\bar{a}^3$, respectively, and 1 G = 0.1 mT. (Finally, $\bar{a} = 42.95a_0$, $61.65a_0$, $43.63a_0$, and $96.51a_0$ for ^{23}Na, ^{39}K, ^{52}Cr, and ^{133}Cs, respectively.)

	B_0	$a_{\rm bg}$	$s_{\rm res}$	$V_{\rm q}$	$g_{\rm q}$	$a_{\rm q}$	α	β
^{39}K	745	−0.541	0.00062	4.7	−1540	−0.55	0.0354	0.0468
^{133}Cs	227	21.34	0.19	1000	−4.19	29	−3.55	−3.85
^{23}Na	853	1.47	0.0002				0	0
^{52}Cr	500	2.45	0.03				0	0
^{133}Cs	19.8	1.66	0.002				0	0

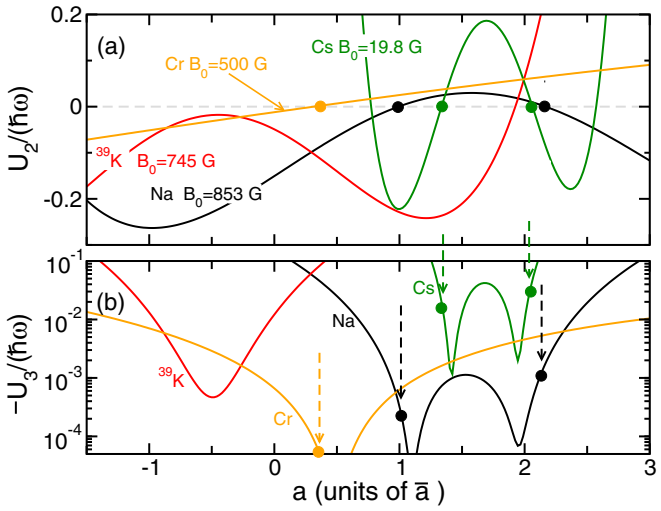

FIG. 4. (a) Two-body interaction strength U_2 and (b) minus one times the three-body strength $-U_3$ in a harmonic trap with $\omega/(2\pi) = 50$ kHz as a function of the scattering length a for a narrow ^{23}Na (black lines), ^{39}K (red lines), ^{52}Cr (orange lines), and ^{133}Cs (green lines) Feshbach resonance tabulated in Table I. Solid circles in both panels and arrows in (b) indicate where $U_2 = 0$.

resonances (with $s_{\rm res} \ll 0.1$) tabulated in Table I and assuming a harmonic trap with frequency $\omega/(2\pi) = 50$ kHz. For all four resonances $U_2 = 0$ for at least one value of a. The second, broader ^{133}Cs resonance with $B_0 = 227$ G and $s_{\rm res} = 0.19$ has no such point and is not shown. The cases where both $U_2 = 0$ and $|U_3|/(\hbar\omega) \ll 1$ are indicated in the figure with markers. For the Na and Cs resonances $U_2 = 0$ when $a \approx \bar{a}$ or $2\bar{a}$ and $-U_3/(\hbar\omega) \geqslant 0.001$. For the ^{39}K resonance a zero crossing occurs at $a \approx 2\bar{a}$ but $U_3/(\hbar\omega) \gg 1$, outside the validity range of the theory.

Finally, we compare the expected value of U_3 with the tunneling energy J, depicted in Fig. 1, in an optical lattice. Noting that for commonly used lasers in and near the optical domain the recoil energy E_R/h lies between 2 and 10 kHz for alkali-metal atoms, we find that for $\omega/(2\pi) = 50$ kHz the tunneling energy J is about ten times smaller than $|U_3|$. For a shallower lattice and thus smaller ω the tunneling energy increases exponentially, while U_3, maintaining the condition that $U_2 = 0$, decreases much more slowly.

VI. DETECTION AND THREE-BODY RECOMBINATION

Several observations can be made about the feasibility and limitations of the proposal. These range from the detection of the point where $U_2 = 0$, the behavior of Bose-Hubbard models, and three-body recombination. The next two sections briefly address these points.

A. Detection of $U_2 = 0$?

We can locate lattice parameters where $U_2 = 0$ with two types of experiments. The simplest is to perform vibrational spectroscopy on two or three isolated bosonic atoms held in a dipole trap or in an optical lattice where tunneling is negligible. For pairs of fermionic alkali-metal atoms as well as for one fermion and one boson in an optical lattice site this has been shown to work near a Feshbach resonance by Refs. [59,60]. Based on predictions of Ref. [61] they found a new class of confinement-induced bound states for large scattering lengths. An accurate study for smaller scattering lengths on the order of the mean scattering length or less, however, is lacking for both fermionic and bosonic alkali-metal atoms. For ^{88}Sr with its small, negative scattering no such measurements have been performed. Finally, no spectroscopic experiments for three atoms exist.

A second type of experiments that can locate $U_2 = 0$ are so-called collapse-and-revival experiments in optical lattices, where changes of the lattice parameters induce nonequilibrium dynamics. Specifically, realizations where after a sudden and large increase of the lattice depth tunneling is negligible, the values for U_2 and U_3 can be inferred from measurements of the momentum distribution as a function of delay after the ramp [37,62–64]. In these experiments the initial state is a superfluid and, hence, to good approximation each site contains a superposition of atomic Fock states in the lowest trap level. After the sudden lattice-depth increase this superposition starts to evolve and measurement of the momentum distribution is sensitive to differences of the energies E_n for different n. These measurements have not been repeated near Feshbach resonances.

B. Three-body recombination

Atom loss from the lattice can limit the realization of our proposal. Loss of one atom at a time, due to collisions with background molecules in the vacuum or light-induced loss from the lattice lasers, can be mitigated by improving the vacuum pressure and a careful choice of laser frequencies. Two-body loss can always be removed by choosing the hyperfine state with the lowest internal energy. This leaves inelastic three-body recombination as an intrinsic loss mechanism. An ultracold homogeneous thermal gas with number density n loses atoms according to the rate equation $dn/dt = -3K_3n^3$. For scattering from short-range potentials [23,65] the event rate coefficient $K_3 \leqslant C_{\rm max}\hbar a^4/m$ with $C_{\rm max} = 67$ when the scattering length $|a| \gg \bar{a}$, while $K_3 \approx C_0\hbar\bar{a}^4/m$ with $C_0 = 25$ for $|a| \sim \bar{a}$. Recently, Refs. [25,26] showed that for longer-ranged van der Waals potentials and near collisional resonances C_0 depends on atomic species and resonance and can be much larger than 25. Finally, Ref. [27] showed empirically that for a broad ^{7}Li resonance with a negative effective range $K_3 \approx C_{\rm max}\hbar(a^3 - r_e a^2/2)^{4/3}/m$ gives a reasonable description of experimental data close to the resonance.

In a lattice site recombination can be included as an imaginary contribution to U_3. That is, we use $U_3 \to U_3 - i\Gamma_3/2$, where $\Gamma_3 = \hbar K_3 \int d^3\vec{x}|\Psi(\vec{x})|^6$ and $\Psi(\vec{x})$ is the normalized single-atom ground-state wave function in a lattice site. For an isotropic harmonic trap and $|a| \sim \bar{a}$ this leads to

$$\Gamma_3 = \frac{C_0}{3\pi^3}\frac{\bar{a}^4}{\ell^4}\hbar\omega \tag{12}$$

when $U_2 = 0$. Losses are acceptable when $\Gamma_3 \ll |U_3|$ and thus

$$\frac{|a|}{\bar{a}} \gg \sqrt{\frac{3\sqrt{3}C_0}{32\pi^2}}\frac{\bar{a}}{\ell} = 0.64\frac{\bar{a}}{\ell} \tag{13}$$

for $C_0 = 25$. Since typically $\ell > 10\bar{a}$, a scattering length on the order of $\bar{a}$ is required. This condition can be met with Feshbach resonances but also indicates that an experiment with ^{88}Sr will be hard. A similar analysis with a more restrictive estimate of Ref. [27] suggests that weaker trapping potentials with $\ell \gg 10\bar{a}$ will be required.

VII. CONCLUSION

We have proposed a means to create an ultracold gas of bosonic atoms in an optical lattice that only interacts via on-site three-body interactions. This is achieved by a careful cancellation of two contributions in the pairwise interaction between two atoms, one proportional to the zero-energy scattering length and a second proportional to the effective range. We predict that this cancellation can occur for the strontium-88 isotope as well as near narrow magnetic Feshbach resonances in alkali-metal atoms or chromium collisions.

For optical lattice depths and/or magnetic field strengths where the pairwise interaction has been canceled, i.e., $U_2 = 0$, we have also shown that the three-body interaction strength can be of the same order of magnitude as the tunneling energy of atoms hopping between neighboring lattice sites. Three-body recombination can limit the practical duration of coherent atom evolution.

Although the purpose of this paper has not been the characterization of the many-body ground state or the dynamical properties of a system near $U_2 = 0$, a brief remark is in order. For a small number of atoms per lattice site we predict that the three-body interaction is attractive. For a Hubbard model with finite tunneling J on the order of U_3 this can indicate that the ground state corresponds to a state with all atoms in one site and, in essence, the system would "collapse," similar to the instability of systems with a negative two-body strength U_2. To prevent this collapse a weak global trapping potential must be added. On the other hand, we expect that it is realistic to perform dynamical experiments where initially the ground state for positive U_2 is prepared and, subsequently, the lattice parameters are changed to ones where $U_2 = 0$.

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