Atomic Quantum Gases in Kagomé Lattices

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We demonstrate the possibility of creating and controlling an ideal and *trimerized* optical Kagomé lattice, and study the low temperature physics of various atomic gases in such lattices. In the trimerized Kagomé lattice, a Bose gas exhibits a Mott transition with fractional filling factors, whereas a spinless interacting Fermi gas at 2/3 filling behaves as a quantum magnet on a triangular lattice. Finally, a Fermi-Fermi mixture at half-filling for both components represents a frustrated quantum antiferromagnet with a resonating-valence-bond ground state and quantum spin liquid behavior dominated by a continuous spectrum of singlet and triplet excitations. We discuss the method of preparing and observing such a quantum spin liquid employing molecular Bose condensates.

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During the past 30 years, condensed matter physics has devoted considerable interest to the issue of frustrated quantum antiferromagnets (QAF) (cf. [1]). In 1973, Anderson proposed [2] the resonating-valence bond (RVB) for the ground state of QAFs, where all spins are paired into singlets. RVB states exhibit neither the standard antiferromagnetic Néel order nor the spin-Peierls order (for which singlet pairs are ordered in space). Recent extensive numerical studies have shown that the RVB physics characterizes the spin 1/2 Heisenberg antiferromagnet on the 2D Kagomé lattice in 2D [see Fig. 1(a)] [3,4]. The spectrum of this system has a very peculiar structure: The energy gap between the ground state and the lowest triplet state, if any, is predicted to be very small (of order $J/20$, where J is the spin exchange coupling). This gap is filled with low-lying singlet states. Their number scales as 1.15^N with the number of lattice sites N. For temperatures above the triplet gap, the spin correlations decay rapidly in space, but have a very slow temporal behavior $\langle s(x,0)s(x,t)\rangle \propto 1/t^{0.6}$ [5].

A very illuminating analytic insight into the physics of QAF in the Kagomé lattice has been recently obtained by Mila and Mambrini [6], who considered a trimerized Kagomé lattice (TKL) [see Fig. 1(b)]. Such a lattice is a triangular lattice of trimers with intra(inter)trimer couplings J and $J' \ll J$, respectively. In Refs. [6], a nontrivial mean-field theory has been formulated that predicts correctly the number, the form, and the spectrum of singlet excitations, which correspond to a restricted set of short-range RVB states. For $J' \ll J$, the theory predicts a triplet gap $(2/3)J'$. All these theoretical findings do not yet have a clear experimental confirmation in condensed matter systems, and it is thus desirable to seek other possible testing grounds.

Such novel testing grounds could be provided by the atomic physics of ultracold quantum lattice gases, which is one of the most rapidly developing fields of alternate molecular orbital physics nowadays. Following the proposal of Jaksch *et al.* [7], Greiner *et al.* [8] were the first to demonstrate the superfluid-Mott insulator (MI) transition in a lattice Bose gas, predicted earlier in Ref. [9]. Atomic physics and quantum optics offer in this context a new and very precise way of preparing, manipulating, and detecting the system under investigation.

In this Letter we show that, using superlattices techniques [10], it is possible to create a 2D optical trimerized Kagomé lattice, and to control in real time the degree of trimerization (i.e., the ratio of J'/J). The physics of cold atomic gases in such an optical lattice is described quite

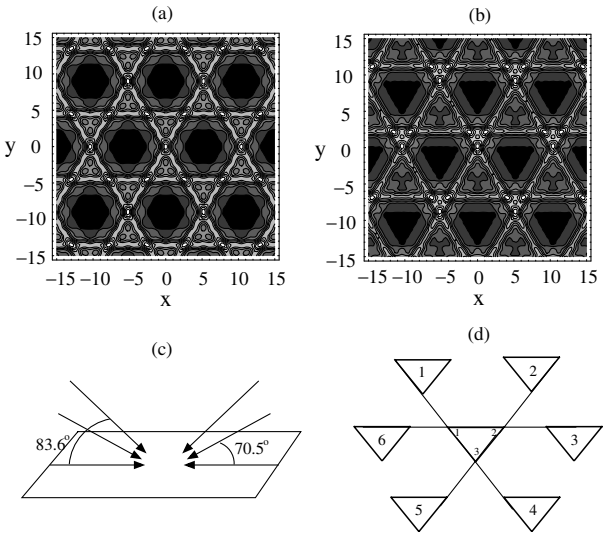

FIG. 1. (a) Ideal Kagomé lattice for $\phi = \pi/2$. (b) TKL using $\phi = \pi/4$. This lattice can be generated using three SWs with a $\pi/3$ angle between themselves. Each SW is generated by three lasers with a configuration shown in (c). (d) Enumeration of spins in a trimer and of neighboring trimers.

generally by various versions of the Hubbard model, and the energies and couplings defining such models can be calculated using solid-state methods (tight binding approximation, Wannier function expansion [11]). Such an unprecedented possibility motivates us to consider three kinds of quantum gases in the TKL: (i) a Bose gas with repulsive interactions; for this case we predict the appearance of Mott-insulator phases with fractional fillings $\nu = 1/3, 2/3$; (ii) a spinless Fermi gas with nearest-neighbor interactions; such gas appears, for instance, naturally as a strong-interaction limit of the Bose-Fermi Hubbard model [12]. In this case, fermions (or, more generally composite fermions consisting of bare fermions coupled to bosons or bosonic holes) attain boson mediated interactions. Interestingly, at $2/3$ filling the Fermi gas behaves as a frustrated quantum magnet on a triangular lattice with couplings dependent on the direction of the bonds. (iii) Finally, we consider a Fermi-Fermi mixture at full total filling $N_1 = N_2 = N/2$, where N_i is the number of fermions of each species. Such a system in the strong coupling limit is equivalent to the spin $1/2$ Heisenberg antiferromagnet in zero magnetic field, and the physics of this system is well described by the RVB model. We discuss in detail how to prepare a system in low-lying singlet states, and how to detect its properties.

In the following, we consider the atoms in a 2D optical lattice in the xy plane, being strongly confined (magnetically or optically) in the z direction. In order to form a Kagomé lattice, one can use blue detuned lasers, so that the potential minima coincide with the laser intensity maxima [13]. A perfect triangular lattice can be created by two standing waves (SWs) on the xy plane, $\cos^2(\vec{k}_{1,2}\vec{r})$, with $\vec{k}_{1,2} = k\{1/2, \pm\sqrt{3}/2\}$, and an additional SW $\cos^2(\vec{k}_3\vec{r} + \phi)$, with $\vec{k}_3 = k\{0, 1\}$. The resulting triangles have a side of length $2\pi/\sqrt{3}k$. By varying ϕ, the third SW is shifted along the y axis, and, in principle, a Kagomé pattern could be realized.

However, three lasers on a plane cannot have a mutually orthogonal polarization, and, hence, undesired interferences between SWs occur. This can be avoided by randomizing the relative orientation of the polarization between SWs, or by introducing small frequency mismatches, which, however, have to be larger than any other relevant frequencies. Moreover, due to diffraction, the ratio ξ between the separation between maxima and the half width at half maximum is 4, and, for any ϕ, the potential minima forming the Kagomé triangles cannot be resolved. This can be avoided by using superlattices. For example, one may substitute each SW ($i = 1, 2, 3$) by a potential $[\cos(\vec{k}_i\vec{r}) + 2\cos(\vec{k}_i\vec{r}/3)]^2$, for which $\xi = 7.6$, and a perfect Kagomé lattice for $\phi = \pi/2$, and a modestly TKL for $5\pi/12 \leq \phi \leq \pi/2$ is possible. For another superlattice [Fig. 1(c)], $[\cos(\vec{k}_i\vec{r}) + 2\cos(\vec{k}_i\vec{r}/3) + 4\cos(\vec{k}_i\vec{r}/9)]^2$, with $\xi \sim 14$, one can reach a strongly TKL [Fig. 1(b)].

The proposed scheme allows one to realize the trimerized and the ideal Kagomé lattice, and transform one into the other and back by changing ϕ. One is thus tempted to study the physics of ultracold gases in such lattices. In the following, we consider three different physical systems: a Bose gas, a single component Fermi gas with nearest-neighbor interactions, and a two-component Fermi gas. The physics of these systems is quite generally described by a Hubbard model [7]. The parameters of the model include intra(inter)trimer tunneling (hopping) J (J'), on-site interaction energies V for different species, and nearest-neighbor interactions U (U'). These parameters can be controlled in a broad range by modifying the laser detunings and intensities, as well as the configuration of the superlattices (the phase ϕ).

To calculate the parameters $J, J', V, \ldots$, we determine first the Bloch functions for the problem. Since there are three lattice sites per Bravais lattice, the lowest band splits actually into three different bands [11]. For each of the bands we calculate the corresponding Wannier functions (localized at each one of the Kagomé triangles), and combine them to construct functions localized at each lattice site. Once these functions are known, the tunneling and interaction coefficients are calculated as in Ref. [7].

We consider first the Bose gas, which is described by the corresponding Bose-Hubbard Hamiltonian:

$$H_{\mathrm{BH}} = -\sum_{\langle ij\rangle}(J_{ij}b_i^\dagger b_j + \mathrm{H.c.}) + \sum_{\langle ij\rangle}U_{ij}n_in_j + \sum_i[Vn_i(n_i-1)/2 - \mu n_i], \quad (1)$$

where the tunneling and nearest-neighbor interaction coefficients J_{ij} and U_{ij} take here the values J and U for intratrimer, and J' and U' for intertrimer hopping, μ is the chemical potential, $n_i = b_i^\dagger b_i$, and $b_i, b_i^\dagger$ are the annihilation and creation operators for bosons at the site i. In the limit when the boson number $N_B \leq N$, i.e., for filling factors $\nu \leq 1$, and for strong on-site interactions $V \gg J, J'$, only one particle may occupy a lattice site.

In the strongly trimerized case ($J', U' \ll U < J$), the system will enter a trimerized Mott phase with the ground state corresponding to the product over (independent) trimers. Depending on the particular value of $\bar{\mu} \equiv (\mu - U)/(2J + U)$, we may have 0 ($\bar{\mu} < -1$), one ($-1 \leq \bar{\mu} < 0$), two ($0 \leq \bar{\mu} < 1$), or three ($1 \leq \bar{\mu}$) bosons per trimer, i.e., filling factors $\nu = 0, 1/3, 2/3$, or one boson per site. For fractional filling, the atoms within a trimer minimize the energy forming a, so-called, W state [14]: $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ for $\nu = 1/3$, and $|W\rangle = (|110\rangle + |101\rangle + |011\rangle)/\sqrt{3}$ for $\nu = 2/3$. It is worth noticing that W states themselves have interesting applications for quantum information theory (cf. [15]).

Generalizing the Landau mean-field theory of Ref. [9], we obtain the phase diagram in the $\bar{J}' \equiv J'/(2J + U)$ and $\bar{\mu}$ plane with characteristic lobes describing the boundaries of the Mott phases, given by $\bar{J}' = (|\bar{\mu}| - 1)/2$ for $|\mu| \geq 1$, and $\bar{J}' = (3/2)|\bar{\mu}|(1 - |\bar{\mu}|)/(4 - |\bar{\mu}|)$ for $|\mu| < 1$. Observations of this Mott transition require

temperatures T of the order of J', i.e., smaller than J and U. Assuming U of the order of few recoil energies [8], that implies T in the range of tens of nK. The results for $J < U$ are qualitatively similar. Note that direct monitoring of the number of particles per trimer is feasible; also, time-of-flight experiments should reveal the coherence of the W states.

The spinless Fermi gas in the trimerized Kagomé lattice is described by the Fermi-Hubbard Hamiltonian:

$$H_{\mathrm{FH}} = -\sum_{\langle ij\rangle}(J_{ij} f_i^\dagger f_j + \mathrm{H.c.}) + \sum_{\langle ij\rangle} U_{ij} n_i n_j - \sum_i \mu n_i, \tag{2}$$

where as before J_{ij} and U_{ij} take the values J and U for intratrimer, and J' and U' for intertrimer hopping, μ is the chemical potential, $n_i = f_i^\dagger f_i$, and $f_i, f_i^\dagger$ are the fermionic annihilation and creation operators. In the following, we enumerate the sites in each trimer 1, 2, and three clockwise starting from the upper left site. We denote the three different intratrimer modes by $f = (f_1 + f_2 + f_3)/\sqrt{3}$ (zero momentum mode), and $f_\pm = (f_1 + z_\pm f_2 + z_\pm^2 f_3)/\sqrt{3}$ (left and right chirality modes), where $z_\pm = \exp(\pm 2\pi i/3)$. The intratrimer Hamiltonian acquires the form $H_{\mathrm{intra}} = -3Jf^\dagger f + U[(\bar{n} - \tilde{\mu})^2 - \tilde{\mu}^2]/2$, where $\bar{n}$ is the total fermion number in the trimer, whereas $\tilde{\mu} = (\mu - J + U/2)/U$. In the strongly trimerized limit, we have (depending on the value of $\tilde{\mu}$): 0 ($\tilde{\mu} < 1/2 - 3J/U$), one ($1/2 - 3J/U < \tilde{\mu} < 3/2$), two ($3/2 < \tilde{\mu} < 5/2$), or three ($\tilde{\mu} > 5/2$) fermions per trimer. Obviously, the cases with zero and three fermions per trimer are not interesting. For one fermion per trimer or less (filling factor $0 \le \nu \le 1/3$), at low temperatures ($T < J$) the fermions will preferably occupy the lowest energy zero momentum mode f forming a gas of f fermions on a triangular lattice, with a tunneling rate $J'/3$, and a coupling constant for nearest-neighbor interactions $U'/9$. Depending on the sign of U', we expect a similar behavior as in Ref. [12], i.e., the appearance of a superfluid phase or fermionic domains for $U' < 0$, and Fermi liquid, or density wave phases for $U' > 0$.

The situation is more complex in the case of two fermions per trimer, since the second fermion may then have left or right chirality, while the first fermion occupies the f state with certainty. The system becomes equivalent to a quantum magnet with interactions that depend on the bond directions:

$$H_{\mathrm{int}} = \frac{2U'}{9}\sum_i \sum_{j=1}^{6} s_i(\phi_{i\to j}) s_j(\tilde{\phi}_{j\to i}), \tag{3}$$

where nearest neighbors are enumerated as shown in Fig. 1(d). In Eq. (3), we have $s(\phi) = \cos(\phi)s_x + \sin(\phi)s_y$, where $s_x = (f_+^\dagger f_- + f_-^\dagger f_+)/2$ and $s_y = -i(f_+^\dagger f_- - f_-^\dagger f_+)/2$. The angles ϕ are $\phi_{i\to 1} = \phi_{i\to 6} = 0$, $\phi_{i\to 2} = \phi_{i\to 3} = 2\pi/3$, $\phi_{i\to 4} = \phi_{i\to 5} = -2\pi/3$, $\tilde{\phi}_{1\to i} = \tilde{\phi}_{2\to i} = -2\pi/3$, $\tilde{\phi}_{3\to i} = \tilde{\phi}_{4\to i} = 0$, and $\tilde{\phi}_{5\to i} = \tilde{\phi}_{6\to i} = 2\pi/3$.

The couplings between the left and right modes are effectively ferromagnetic for $U' > 0$, and antiferromagnetic otherwise. Intertrimer hopping J' contributes first in order $(J')^2/U$, and is neglected here. For $U' < 0$, the classical approximation yields a Néel-type ground state with planar order in which on every triangle there is exactly one spin along the $\Phi = 0, 2\pi/3, -2\pi/3$ directions. The excitation spectrum is expected to be gapped. For $U' > 0$, one finds two types of ground states which are degenerate in the classical limit: a planar state of the type just described, but with opposite chirality, and a ferromagnetic state in which the spins align in the xy plane. A linear spin-wave analysis yields a lower energy for the ferromagnetic state. In this approximation the continuous degeneracy of the classical ferromagnet is lifted leaving six degenerate ground states in which the spins align parallel or antiparallel to the three lattice directions. A numerical study of the original spin-1/2 model, Eq. (3), aiming at a check of these semiclassical results is in progress.

The observation of the quantum phases in this model requires $U' < J, U$, and $T < U'$. If the fermionic interactions are due to dipolar forces [16], then U may be of the order of a few recoils, and T in the range of 10–100 nK. If fermionic interactions are due to hopping induced effects in a Bose-Fermi mixture, then T in the range of 10 nK will be necessary (for details, see [12]).

Finally, we consider a Fermi-Fermi mixture with half-filling for each species, i.e., a spin 1/2 Hubbard model:

$$H_{\mathrm{FF}} = -\sum_{\langle ij\rangle} J_{ij}(f_i^\dagger f_j + \tilde{f}_i^\dagger \tilde{f}_j + \mathrm{H.c.}) + \sum_i V n_i \tilde{n}_i, \tag{4}$$

where the operators f_i and $f_i^\dagger$ ($\tilde{f}_i$ and $\tilde{f}_i^\dagger$) are the creation and annihilation operators for the two components, $n_i = f_i^\dagger f_i$ ($\tilde{n}_i = \tilde{f}_i^\dagger \tilde{f}_i$), and, as above, $J_{ij} = J_0$ (J_0') for intra(inter)trimer hopping. In the strong coupling limit, $J_0, J_0' \ll V$ (t-J model) [1], H_{FF} reduces to the Heisenberg antiferromagnet,

$$H = J\sum_{\langle i,j\rangle_{\mathrm{intra}}} \vec{s}_i \cdot \vec{s}_j + \bar{J}' \sum_{\langle i,j\rangle_{\mathrm{inter}}} \vec{s}_i \cdot \vec{s}_j, \tag{5}$$

where $J = 4J_0^2/V$, $J' = 4J_0'^2/V$, and $\vec{s} = (s_x, s_y, s_z)$, with $n - \tilde{n} = 2s_z$, $f^\dagger \tilde{f} = s_x + is_y$, and $\tilde{f}^\dagger f = s_x - is_y$.

In the strongly trimerized limit [6], the total spin in the trimer takes the minimal value, i.e., 1/2, and there are four degenerate states having $s_z = \pm 1/2$ and left or right chirality. The spectrum of the system in the singlet sector consists of a narrow band of low energy states of the width of order J', separated from the higher singlet (triplet) bands by a gap of order $3J/4$ ($2J'/3$).

Assuming that we can prepare the system in a singlet state at $J' < T < J$, then the density of states of the low lying singlet levels can be obtained by repeated measurements of the system energy. The latter can be achieved by simply releasing the lattice so that, after taking care of the zero point energy, all of the interaction energy transforms into kinetic energy. Similarly, we can measure the

mean value and the distribution of any nearest-neighbor two-spin correlations. To this aim, one has to apply at the moment of the trap release a chosen nearest-neighbor two-spin Hamiltonian and keep it acting during the cloud expansion (for details, see [17]). In a similar manner, we can measure the spectrum of triplet excitation, by exciting a triplet state, which can be done by flipping one spin using a combination of superlattice methods and laser excitation [18]. The measurement of the singlet-triplet gap requires a resolution better than J'.

A similar type of measurement can be performed in ideal Kagomé lattices, when $J = J'$, for which the singlet-triplet gap is filled with singlet excitations [3]. By varying ϕ, one can transform adiabatically from strongly TKL to ideal Kagomé, for which the final J will be smaller than the initial J, but larger than the initial J'. In that case, the system should remain within the lowest set of 1.15^N states that originally formed the lowest singlet band. The singlet-triplet gap, if any, is estimated to be $\leq J/20$, and should be measurable using the methods described above.

A possible way to prepare a singlet state in the TKL with $T < 3J/4$ could employ the recently obtained Bose-Einstein condensates of molecules consisting of two fermionic atoms [19] at temperatures of the order of 10 nK. Such Bose-Einstein condensates (BECs) should be loaded onto an ideal and weak Kagomé lattice. Note that the molecules formed after sweeping across a Feshbach resonance are in a singlet state of the pseudospin $\vec{s}$. This can easily be seen, because the two fermions enter the resonance from the s-wave scattering channel (i.e., in the symmetric state with respect to the spatial coordinates), and, thus, are in a singlet state of the pseudospin (i.e., antisymmetric state with respect to exchange of electronic and nuclear spins). Since the interaction leading to the spin flipping at the Feshbach resonance [20] is symmetric under the simultaneous interchange of both nuclear and electronic spin, then the formed molecule remains in a pseudospin singlet. The typical size of the molecule is of the order of the s-wave scattering length a, and thus can be modified at the resonance [21], being chosen comparable to the lattice wavelength. Growing the lattice breaks the molecule into two separate fermionic atoms in neighboring sites in the singlet pseudospin state. In this way, a singlet covering of the Kagomé lattice may be achieved, allowing for the direct generation of a RVB state [2].

In summary, we have shown that by employing currently available superlattice techniques it is possible to create in a controlled way a trimerized Kagomé lattice. An ultracold Bose gas in such a lattice exhibits novel Mott insulator phases with fractional filling $\nu = 1/3, 2/3$. A single-component Fermi gas with nearest-neighbor interactions for $\nu = 1/3$ behaves as a Fermi gas in the underlying triangular lattice, whereas for $\nu = 2/3$ it becomes a nonstandard ferromagnet or antiferromagnet in the triangular lattice with direction dependent bonds. Finally, for a Fermi-Fermi mixture in a Kagomé lattice, which is described by an antiferromagnetic Heisenberg model, we have shown the possibility to measure the spectral properties of the latter system. This opens the way for analyzing in a novel and fascinating setting one of the paradigmatic problems of condensed-matter physics, the physics of random valence bond frustrated QAF's.

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