Atomic Quantum Simulator for Lattice Gauge Theories and Ring Exchange Models

H. P. Büchler,[1,2] M. Hermele,[3] S. D. Huber,[4] Matthew P. A. Fisher,[5] and P. Zoller[1,2]

[1]*Institute for Quantum Optics and Quantum Information of the Austrian Academy of Science, 6020 Innsbruck, Austria*
[2]*Institut für theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria*
[3]*Department of Physics, University of California, Santa Barbara, California 93106, USA*
[4]*Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland*
[5]*Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA*

We present the design of a ring exchange interaction in cold atomic gases subjected to an optical lattice using well-understood tools for manipulating and controlling such gases. The strength of this interaction can be tuned independently and describes the correlated hopping of two bosons. We discuss a setup where this coupling term may allow for the realization and observation of exotic quantum phases, including a deconfined insulator described by the Coulomb phase of a three-dimensional U(1) lattice gauge theory.

Loading cold atomic gases into optical lattices allows for the realization of bosonic and fermionic Hubbard models, and offers the possibility for the experimental study of strongly correlated systems within a highly tunable environment. Starting from the prediction of a superfluid to Mott-insulator phase transition in bosonic atomic gases [1] and the subsequent observation of the Mott insulating phase [2–4], many new tools for manipulating and controlling quantum gases have been developed [5]. In this Letter, we combine these tools in order to drive the atomic gas with an additional ring exchange interaction. We identify a promising system where this coupling may allow for the realization and observation of an exotic quantum insulator [6,7] described by the Coulomb phase of a three-dimensional U(1) lattice gauge theory [8]; in quantum magnetism this phase is known as a U(1) spin liquid.

Recently, studies of boson models with large ring exchange have yielded significant progress in the search for microscopic Hamiltonians exhibiting exotic phases [9–11]. This search has been the focus of much effort in two-dimensional systems due to potential relevance for high-T_c cuprates. Some ring exchange models exhibit a local conservation law and can be mapped onto lattice gauge theories and often also quantum dimer models (QDM) [12]. A number of such models in two and three dimensions have been shown to possess deconfined insulating ground states [13]. Many of the three-dimensional models, including those of Refs. [6,7], were shown to possess a U(1) deconfined phase, which supports gapped half-boson excitations, gapped "magnetic monopole" topological defects, and a linearly dispersing photon mode with two polarizations. The low-energy theory is standard quantum electrodynamics with massive electrically and magnetically charged scalar particles. Models of bosons on the square lattice with large ring exchange are in a different class from those above, and also exhibit interesting physics. Such models can support an "exciton Bose liquid" phase, a two-dimensional analog of a Luttinger liquid [14], as well as nontrivial valence-bond solid (VBS)

insulating states [15]. Such states can undergo a direct quantum phase transition to the superfluid [16].

Despite much recent theoretical progress, clear experimental evidence for the existence of exotic phases is still missing. Furthermore, relatively few theoretical techniques exist to study such strongly correlated systems; perhaps the most powerful to date is quantum Monte Carlo simulation, but the class of models that can be productively studied is severely limited by the notorious sign problem. Atomic gases offer an alternative approach through the design of *quantum simulators*, where a microscopic Hamiltonian is implemented in a quantum gas and its phase diagram is studied experimentally via controlling the strength of the interaction terms.

In this Letter, we present the design of a ring exchange interaction for bosonic gases subjected to an optical lattice. Such an atomic lattice gas is well described by the Bose-Hubbard model [1]

$$H_{\mathrm{BH}} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i b_i^\dagger b_i^\dagger b_i b_i, \qquad (1)$$

where U denotes the on-site repulsion and J is the hopping energy with $\langle i, j \rangle$ denoting summation over nearest-neighbor sites. The additional ring exchange interaction involves four lattice sites forming a square plaquette, and is driven by a resonant coupling of the bosons via a Raman transition to a "molecular" two-particle state [5]; see Fig. 1. This state is subjected to an independent optical lattice with its lattice sites at the plaquette centers. The symmetry of the molecular state strongly influences the coupling; we are interested in a d-wave symmetry of the molecule, which can be carried either by the relative coordinate or the center of mass motion. Then, the coupling to the molecular state (created by $m_\square^\dagger$) takes the form

$$H_{\mathrm{M}} = \sum_\square \nu m_\square^\dagger m_\square + g \sum_\square [m_\square^\dagger (b_1 b_3 - b_2 b_4) + \mathrm{H.c.}]. \quad (2)$$

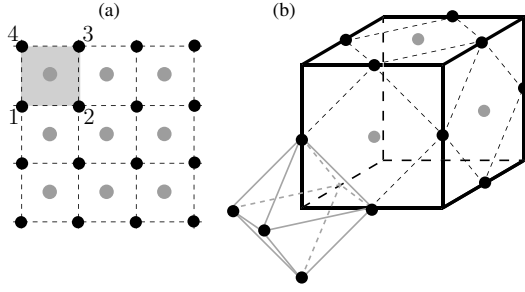The summation runs over all plaquettes $\square$. The single-

FIG. 1. (a) Two-dimensional setup: the bosons (black dots) are on the square lattice with the molecules (gray dots) in the center of each plaquette. (b) Three-dimensional setup: the bosons (black dots) are on the links of the cubic lattice. Within each face there are four bosonic sites, which establish a plaquette (dashed square). The molecules (gray dots) are in the center of each plaquette.

particle states created by $b_i^\dagger$ are called bosonic or atomic states to distinguish them from the molecular two-particle states. Depending on the setup, the atomic states reside either in the corners or on the edges of each plaquette (see Fig. 1), and are numbered counterclockwise. The energy ν corresponds to the detuning from resonance, while g is the coupling strength determined by the Rabi frequency of the Raman transition. While the Hamiltonian (2) is interesting in its own right, the connection to ring exchange is apparent upon integrating out the molecular field perturbatively in g/ν, which leads to the effective Hamiltonian

$$H_{\rm RE} = K \sum_\square (b_1^\dagger b_2 b_3^\dagger b_4 + b_1 b_2^\dagger b_3 b_4^\dagger - n_1 n_3 - n_2 n_4), \quad (3)$$

with $K = g^2/\nu$. Note that the structure of the coupling in Eq. (2) also produces a next-nearest-neighbor interaction. The bosonic system turns metastable for large negative detuning. However, the decay time easily exceeds typical experimental time scales of atomic gases. Then, the perturbative expansion is again valid and allows for the realization of a system with negative ring exchange interaction.

In the following, we present the microscopic design of the ring exchange interaction within atomic gases. This design combines standard tools for manipulating and controlling cold atomic gases [5,17]. Our starting point is a system of bosonic atoms with two internal states coupled via a Raman transition. These different internal states can be trapped by independent optical lattices; such independent trapping has been realized recently using spin-dependent optical lattices [18,19]. An alternative approach is the trapping of alkaline earth metals, e.g., ^{88}Sr, where the first excited state $^3P_1$ exhibits a long lifetime with a different polarizability than the lowest energy state $^1S_0$ [20]. We introduce the notation $\psi_a(\mathbf{x})$ and $\psi_b(\mathbf{x})$ for the field operators describing the two internal states, and the microscopic Hamiltonians then take the form ($\alpha = a, b$)

$$H_\alpha = \int d\mathbf{x}\left[\psi_\alpha^\dagger\left(\frac{-\hbar^2\nabla^2}{2m} + V_\alpha + e_\alpha\right)\psi_\alpha + \frac{g_\alpha}{2}\psi_\alpha^\dagger\psi_\alpha^\dagger\psi_\alpha\psi_\alpha\right],$$

with $g_\alpha = 4\pi\hbar^2 a_\alpha/m$ the interaction strength for scattering lengths a_α. The interaction strengths between the atoms can be tuned independently by using magnetic or optical Feshbach resonances [5]. The e_α are the homogeneous energy shifts between the internal states. The potential $V_\alpha(\mathbf{x})$ accounts for an optical lattice driven by lasers with wave vector $k = 2\pi/\lambda$, with the strength v_α in units of the recoil energy $E_r = \hbar^2 k^2/2m$. The two internal states are coupled via a Raman transition. Transforming away the optical frequencies within a rotating frame, the coupling takes the form

$$H_R = \hbar\Omega \int d\mathbf{x}[\psi_b^\dagger\psi_a + \psi_a^\dagger\psi_b], \quad (4)$$

with Ω the Rabi frequency of the transition.

We focus first on the two-dimensional setup shown in Fig. 1(a). Confinement to two dimensions is achieved by a strong transverse optical lattice, which quenches hopping between different planes. The remaining optical lattice provides the square lattice structure for the atomic state ψ_b and takes the form $V_b/E_r = v_b[\cos^2(kx/2) + \cos^2(ky/2)]$. For $v_b \gtrsim 1$, the mapping to the Bose-Hubbard model is well justified. The optical lattice for the second internal state ψ_a, which is localized at the plaquette centers, takes the form

$$\frac{V_a}{E_r} = v_a\{[\cos kx - \cos ky]^2 + \sin^2(kx/2) + \sin^2(ky/2)\}.$$

The first term is obtained by interference between standing laser waves along the x and y directions, while the other terms represent a standard square lattice. The different lattice spacing of the two contributions is easily achieved by a finite angle $2\pi/3$ between the interfering beams. We are interested in a strong optical lattice V_a, where tunneling between different wells is quenched, and focus on the energy states within a single well. Then the structure of
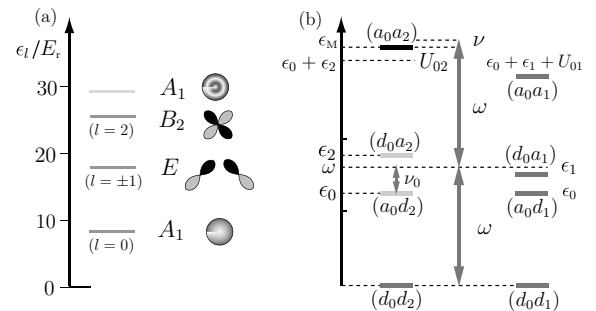

FIG. 2. (a) Single-particle energies ϵ_l of the states $a_{l,\square}^\dagger|0\rangle$ for $v_a = 30$. (b) Energy levels of the two-particle states with symmetry B_2 and E. The frequency $\omega = (\epsilon_0 + \epsilon_2 + U_{02} + \nu)/2\hbar$ of the Raman transition is chosen near resonance with the molecular state $a_0^\dagger a_2^\dagger|0\rangle$ and far detuned to the single-particle excitations.

V_a produces strong shifts of the energy states compared to those obtained within a harmonic approximation. The states are characterized by the irreducible representations of the symmetry group C_{4v} (i.e., the point group of the square lattice); the low-energy states and corresponding representations derived within a band structure calculation are shown in Fig. 2 for $v_a = 30$. The state with energy ϵ_l in each plaquette $\square$ is created by the bosonic operator $a^\dagger_{l,\square}$ with $l = 0, \pm 1, 2$. Of particular interest is the state $|a_{2,\square}\rangle$ corresponding to the representation B_2, which transforms under C_{4v} like the polynomial xy (i.e., d_{xy} symmetry). In contrast to the harmonic approximation, this state is nondegenerate.

For weak interactions, the Hamiltonian for the bosonic field ψ_a reduces to

$$H_a = \sum_{l,\square} \nu_l a^\dagger_{l,\square} a_{l,\square} + \sum_{l,l',\square} \frac{U_{l,l'}}{2} a^\dagger_{l,\square} a^\dagger_{l',\square} a_{l,\square} a_{l',\square}, \quad (5)$$

with $U_{l,l'} \lesssim \epsilon_l$ the interaction energy and $\nu_l = \epsilon_l - \hbar\omega$ the energies of the excitations within the rotating frame (ω is the frequency of the Raman transition). The coupling driven by the Raman transition takes the form $H_R = \hbar\Omega\Sigma_{l,\square}[w_l a^\dagger_{l,\square} d_{l,\square} + \text{H.c.}]$, with Ω the Rabi frequency. Because of the square symmetry, each operator $a_{l,\square}$ couples to a special structure of surrounding bosons. The operators for which the coupling becomes diagonal transform irreducibly under C_{4v} and are $d_{0,\square} \sim b_1 + b_2 + b_3 + b_4$, $d_{\pm 1,\square} \sim b_1 \pm ib_2 - b_3 \mp ib_4$, and $d_{2,\square} \sim b_1 - b_2 + b_3 - b_4$. The wave function overlaps w_l derive from the shape of the localized wave functions. For typical parameters ($v_b \approx 6$ and $v_a \approx 30$) we obtain $w_l \approx 0.1$.

We are interested in a setup with molecular two-particle states $|m_\square\rangle = m^\dagger_\square|0\rangle = a^\dagger_{2,\square} a^\dagger_{0,\square}|0\rangle$ (with d_{xy} symmetry B_2) resonantly coupled to the bosonic states $b^\dagger_i b^\dagger_j|0\rangle$ with detuning ν. The energy of this state is $\epsilon_M = \epsilon_0 + \epsilon_2 + U_{02}$. As the formation of the molecule involves the virtual creation of a single-particle excitation $a^\dagger_{l,\square}|0\rangle$, the frequency of the Raman transition is determined by $\omega = (\epsilon_M + \nu)/2\hbar$ (Fig. 2). We require that the single-particle excitations $a^+_{l,\square}|0\rangle$ are far detuned (i.e., $w_l\hbar\Omega < |\nu_l|$), and only the molecular states are resonantly coupled with $|\nu| \ll |\nu_l|$. As the separation between the energy levels ϵ_l is large ($\sim 2\sqrt{v_a E_r}$), this condition can easily be satisfied for suitable interaction energy U_{02}. Furthermore, it may be of interest to tune the interaction energy via a Feshbach resonance to an optimal value. For such strong interactions the molecular operator becomes $m^\dagger_\square = c_1 a^\dagger_{0,\square} a^\dagger_{2,\square} + c_2(a^\dagger_{1,\square} a^\dagger_{1,\square} + a^\dagger_{-1,\square} a^\dagger_{-1,\square}) + \cdots$, where the ellipsis denotes admixture of higher energy states respecting the d_{xy} symmetry. The parameters $c_{1,2}$ and the energy ϵ_M have to be determined from the solution of the two-particle problem within a single well.

Integrating out the single-particle states $|l, \square\rangle = a^\dagger_{l,\square}|0\rangle$ perturbatively in $\hbar\Omega/\nu_l$, we obtain the effective

Hamiltonian H_M; see Eq. (2). The last term in Eq. (2) accounts for the coupling between molecules $|m_\square\rangle$ and the atomic states $|b_i\rangle$. The operator $b_1 b_3 - b_2 b_4$ is the only second-order polynomial in b_i transforming in the same representation B_2 as the d-wave molecule $|m_\square\rangle$. The coupling g is

$$g = -\hbar^2\Omega^2\left[c_1 w_0 w_2\left(\frac{1}{\nu_0} + \frac{1}{\nu_2}\right) + c_2 w_1^2 \frac{1}{\nu_1}\right], \quad (6)$$

which reduces to $g \sim 4\hbar^2\Omega^2 U_{02}/(\epsilon_2 - \epsilon_0)^2$ for weak interactions $U_{02} \ll \epsilon_0$. We have dropped terms $\sim b_i^2$ as we assume that double occupation of the bosonic sites is strongly suppressed by the on-site repulsion U. In addition to the Hamiltonian in Eq. (2), we obtain a laser induced hopping term $\Sigma_{l,\square}J_l d^\dagger_{l,\square} d_{l,\square}$ with $J_l = -\hbar^2\Omega^2|w_l|^2/\nu_l$. The sign of this laser induced hopping depends on the detuning. In principle it is possible to cancel these terms via interference by an additional far-detuned Raman transition. Furthermore, we have absorbed a shift in the energy of the molecular energy into a redefinition of ω. Tuning the Rabi frequency Ω sets the energy scale of the coupling g, while the detuning ν is controlled by the frequency ω of the Raman transition; this allows the system to be tuned through a resonance.

The zero temperature phase diagram of the two-dimensional setup shown in Fig. 1(a) with the Hamiltonian $H = H_{BH} + H_M$ has not yet been studied. However, by considering appropriate limits we suggest there is potential for interesting physics in the intervening regime. We let q be the average number of atoms per unit cell (i.e., molecular states counted twice) and consider the filling $q = 1/2$. For large positive detuning $\nu \gg g$ with $J \gg g^2/\nu$, the system reduces to the conventional Bose-Hubbard model, see Eq. (1), and the bosons establish a superfluid phase due to the incommensurate filling. In the opposite limit of large negative detuning ($|\nu| \gg J, g$ and $\nu < 0$), all bosons are paired into molecules, and we can think in terms of an effective molecular Bose-Hubbard model at $1/4$ filling. For $J \ll g$, perturbation theory in $g/|\nu|$ generates a nearest- and next-nearest-neighbor repulsion between molecules $U_M \sim g^4/|\nu^3|$. Furthermore, a molecular ring exchange term is generated at the same order. The ground state of the resulting model is not known, but is likely to be a molecular charge density wave with $\langle m^\dagger_\square m_\square\rangle$ larger on every other row and column. There is no difference at the level of symmetry between this state and a "plaquette" valence-bond solid (VBS) of the atomic bosons. We therefore suggest that this system is a candidate for a deconfined quantum critical point [16] as the system is tuned between the VBS and the bosonic superfluid.

The above design of a ring exchange interaction for bosonic systems is a building block that can be applied to different setups and lattice structures in two and three dimensions. Of particular interest are models exhibiting a local gauge invariance that may allow for the realization of

deconfined insulators [6]. In the following, we present such a three-dimensional setup that can likely access a U(1) deconfined state.

The lattice structure of this setup is described by a cubic lattice with the bosonic states on the links; see Fig. 1(b). Each cubic face forms a plaquette involving four link bosons created by the operator $b_{ij}^\dagger$. Between these four link bosons we drive a ring exchange interaction via placing a molecular state at the plaquette centers, i.e., in the center of each cubic face. With this definition of the bosonic and molecular sites, we can again derive the Hamiltonian $H = H_{BH} + H_M$ shown in Eqs. (1) and (2). The microscopic derivation of these effective Hamiltonians follows very closely the derivation in the two-dimensional setup: modifications appear only due to the complex lattice structure, which requires a detailed band structure analysis (the details of this design will be presented elsewhere [21]). We expect that the phase diagram of this system is dominated by a superfluid phase for large hopping, while in the limit of small hopping more exotic states may result. To better understand the possibilities, we consider the limit of vanishing hopping $J = 0$. For large detuning $|\nu| \gg g$, the molecules can be integrated out to obtain the cubic ring exchange model of Ref. [6] with an additional interaction term; see Eq. (3). (Note that a unitary transformation allows one to change the sign of the ring exchange term.) This model is a U(1) lattice gauge theory and, at least over some region of the parameter space, it can enter its Coulomb phase, i.e., a U(1) deconfined insulator [6]. It has been shown that this state is stable to *all* perturbations, including those that break the gauge invariance such as a boson hopping J. Then, in the presence of a small but finite hopping J, the gauge structure goes from an explicit, microscopic property to an emergent one present only in the low-energy theory.

Remarkably, the three-dimensional setup shown in Fig. 1 with the Hamiltonian $H = H_{BH} + H_M$ and quenched hopping $J = 0$ is even a U(1) lattice gauge theory for arbitrary g/ν. This can be seen by considering a cubic site i, letting $L(i)$ be the 6 cubic links and $P(i)$ the 12 plaquettes containing i. Then the local object $G_i = \Sigma_{ij \in L(i)} b_{ij}^\dagger b_{ij} + \Sigma_{\square \in P(i)} m_\square^\dagger m_\square$ is a conserved U(1) "gauge charge." A straightforward "spin wave" treatment allows one to write down a low-energy theory of liquid phases in ring exchange models [6,14], and we obtain here an artificial photon mode with two polarizations. This analysis demonstrates that this model is likely to support a U(1) deconfined insulator, which is likely to be continuously connected to the U(1) deconfined phase discussed above and in Ref. [6] for the large-ν limit. We also note that $H = H_{BH} + H_M$ should be amenable to quantum Monte Carlo simulation when $J = 0$, as a simple unitary transformation renders all matrix elements of $e^{-\tau H}$ nonnegative in the number basis.

In conclusion, we have presented an experimentally accessible setup for the design of ring exchange interaction on cold atomic gases. This design offers the possibility for the atomic quantum simulation of a certain class of strong coupling Hamiltonians and opens an alternative approach for the study of novel and exotic phases with strong correlations. In addition, we remark that the *d*-wave molecular state couples to a special structure of the surrounding bosons. It should be possible to use the coupling of this state as a *probe* of this structure within phases of the atomic system. This may provide a powerful tool for the detection of unconventional order in strongly correlated systems.

[1] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).

[2] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) **415**, 39 (2002).

[3] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).

[4] C. D. Fertig, K. M. O'Hara, J. H. Huckans, S. L. Rolston, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. **94**, 120403 (2005).

[5] D. Jaksch and P. Zoller, Ann. Phys. (Berlin) **315**, 52 (2004).

[6] M. Hermele, M. P. A. Fisher, and L. Balents, Phys. Rev. B **69**, 064404 (2004).

[7] R. Moessner and S. L. Sondhi, Phys. Rev. B **68**, 184512 (2003).

[8] J. B. Kogut, Rev. Mod. Phys. **51**, 659 (1979).

[9] R. Moessner and S. L. Sondhi, Phys. Rev. Lett. **86**, 1881 (2001).

[10] L. Balents, M. P. A. Fisher, and S. M. Girvin, Phys. Rev. B **65**, 224412 (2002).

[11] O. I. Motrunich and T. Senthil, Phys. Rev. Lett. **89**, 277004 (2002).

[12] D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61**, 2376 (1988).

[13] T. Senthil, cond-mat/0411275.

[14] A. Paramekanti, L. Balents, and M. P. A. Fisher, Phys. Rev. B **66**, 054526 (2002).

[15] A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, Phys. Rev. Lett. **89**, 247201 (2002).

[16] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Science **303**, 1490 (2004).

[17] L. Santos, M. A. Baranov, J. I. Cirac, H.-U. Everts, H. Fehrmann, and M. Lewenstein, Phys. Rev. Lett. **93**, 030601 (2004).

[18] O. Mandel, M. Greiner, A. Widera, T. Rom, T. W. Hänsch, and I. Bloch, Phys. Rev. Lett. **91**, 010407 (2003).

[19] L.-M. Duan, E. Demler, and M. D. Lukin, Phys. Rev. Lett. **91**, 090402 (2003).

[20] H. Katori, T. Ido, and M. Kuwata-Gonokami, J. Phys. Soc. Jpn. **68**, 2479 (1999).

[21] H. P. Büchler, M. Hermele, S. D. Huber, M. P. A. Fisher, and P. Zoller (to be published).