Orbital order of spinless fermions near an optical Feshbach resonance

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(Dated: January 18, 2013)

We study the quantum phases of a three-color Hubbard model that arises in the dynamics of the p-band orbitals of spinless fermions in an optical lattice. Strong, color-dependent interactions are induced by an optical Feshbach resonance. Starting from the microscopic scattering properties of ultracold atoms, we derive the orbital exchange constants at 1/3 filling on the cubic optical lattice. Using this, we compute the phase diagram in a Gutzwiller ansatz. We find novel phases with ‘axial orbital order’ in which p_x and p_x + ip_y (or p_x - ip_y) orbitals alternate.

PACS numbers: 03.75.Ss, 05.30.Fk, 67.85.-d, 71.10.Fd

Orbital physics of electrons plays an important role in strongly-correlated solid-state systems, e.g., transition-metal oxides (see, e.g., [1][2] and references therein). In particular, intriguing quantum phases emerge due to the coupling of the orbital degree of freedom to the charge, spin, or lattice degrees of freedom [3][4]. Such coupling, while leading to interesting effects, also complicates the theoretical treatment. It is, therefore, desirable to study simpler systems with the orbital degree of freedom decoupled from all others. Ultracold atoms in higher bands of optical lattices provide an ideal tool to study orbital dynamics in a well-controlled environment, including orbital-only models of single-species (spinless) fermions.

Several groups have now achieved loading and manipulating ultracold atoms in higher (such as p-) bands of optical lattices [5][9]. Techniques such as lattice ramping or radio-frequency pulses have been used to transfer atoms from the s- to higher bands, where they can stay in a metastable state for a sufficiently long time. For spinless fermionic atoms, the p-band can also be simply populated by first completely filling the s-band, requiring larger particle numbers, but less experimental control. To avoid undesired collisions between ground and excited-band atoms, the s-band atoms may be removed afterwards using laser pulses [10].

The interaction between fermionic atoms is usually weak at low temperatures because the Pauli exclusion principle only allows scattering in high partial-wave channels (p, f, etc.). One way to increase the p-wave elastic scattering cross section is to employ a Feshbach resonance (FR) [11]. Typically, this is done by coupling channels in the electronic ground state through magnetic fields. For the case of p-waves, however, this method usually leads to significant atom losses through three-body inelastic collisions because the scattering state is well localized by the angular momentum barrier, and has good Franck-Condon overlap with more deeply bound molecules [12]. To circumvent this problem, recently Ref. [13] considered enhanced p-wave interactions via an optical FR (OFR) between a scattering state and an electronically excited “purely-long-range” molecule. Such molecules have inner turning points at very large distances (e.g., > 50a_0 in ^{171}Yb), well beyond the chemical binding region, and thus three-body recombination should be highly suppressed. This approach not only allows to study strongly-correlated phases, but also provides for a high degree of control. In particular, the interaction strength among different p-orbitals can be tuned differently.

Motivated by these developments, we investigate in this article the phase diagram of spinless fermions on a cubic lattice near an OFR described by the following Hubbard-like model:

\[
H = - \sum_{i,\mu,\nu} t_{\mu,\nu} (c_{\mu,i}^\dagger c_{\nu,i} + c_{\nu,i}^\dagger c_{\mu,i} + \text{h.c.}) + \sum_{i} \left[ V_{1} n_{x,i} n_{y,i} + V_{2} (n_{x,i} n_{z,i} + n_{y,i} n_{z,i}) + (i V_{3} c_{x,i}^\dagger c_{y,i} n_{z,i}^\dagger + \text{h.c.}) \right]. \quad (1)
\]

The operator \(c_{\mu,i}\) destroys a fermion in the orbital \(p_{\mu}\) at site \(i\), and \(n_{\mu,i}\) is the corresponding number operator. The lattice spacing is set to 1, \(e_{\nu}\) is the unit vector in direction \(\nu\), and \(\mu, \nu = x, y, z\). The nearest-neighbor hopping amplitude \(t_{\mu,\nu}\) describes hopping of fermions in orbital \(p_{\nu}\) along the direction \(e_{\nu}\). Due to the anisotropy of the p-orbital Wannier wave functions, it is direction and orbital dependent [14][16], \(t_{\mu,\nu} = t_{\parallel} \delta_{\mu,\nu} + t_{\perp} (1 - \delta_{\mu,\nu})\).

The interactions \(V_{1,2,3}\) are induced by an OFR laser [13] which couples the electronic ground state of the atom to an excited state. The interaction can be expressed in terms of the (p-wave) pseudo-potential \(V_{p}^{\text{m}}\) for two particles with mass \(M\) and relative an-
ular momentum \( m \), \( V^m_\mu (r) = \lim_{\rho \to 0} \frac{2\pi \rho}{m^2} \delta(r-s) \rho^2 \).

The real part of the \( p \)-wave scattering volume, \( R = \text{Re} \{ a_\mu^m \} \), can be tuned by the detuning and the intensity of the OFR laser. Expanding field operators in the Wannier basis, \( \psi (r) = \sum_{\mu, \nu} w_{\mu, \nu} (r-i \epsilon_{\mu, \nu}) \), the interaction term \( \int d^2 r_1 \int d^2 r_2 \psi^\dagger (r_1) \psi (r_2) V^\mu_\nu (r_1 - r_2) \psi (r_1) \psi (r_2) \) leads to the on-site, inter-orbital interaction \( H_{\text{int}} = \sum_{\mu, \nu, \mu', \nu'} V_{\mu, \nu, \mu', \nu'} c^\dagger_{\mu, \nu} c^\dagger_{\mu', \nu'} c_{\mu', \nu'} c_{\mu, \nu} \), where repeated indices are summed over. (We neglect all off-site interactions.) The matrix element \( V_{\mu, \nu, \mu', \nu'} = \sum_{\mu} \int d^3 r_1 \int d^3 r_2 w_{\mu} (r_1 - i \epsilon_{\mu, \nu}) V^\mu_\nu (r_1 - r_2) w_{\mu'} (r_2 - i \epsilon_{\mu', \nu'}) \) can now be computed by separating the relative and center-of-mass coordinates. For deep lattices, the \( p \)-orbital Wannier functions are well approximated by the first excited states of harmonic oscillators (with the oscillator length \( \zeta \) controlled by the lattice depth). The only non-zero interaction terms are the ones given in Eq. \( 1 \), with \( V_1 = \frac{1}{2} (U_1 + U_{-1}) \), \( V_2 = \frac{1}{8} (U_1 + U_{-1} + 2U_0) \), and \( V_3 = \frac{1}{8} (U_{-1} - U_1) \). Here, \( U_m = 3\sqrt{2} \nu / (\sqrt{\pi} \zeta^5 M) \) defines the interaction strength in the scattering channel with angular momentum \( m = 1, 0, -1 \). A Zeemann splitting, which may be introduced by a magnetic field, leads to different detuning of the OFR laser for the three scattering channels. This makes the scattering length \( a_\mu^m \) dependent on \( m \), and consequently the \( U_m \)'s can be different in magnitude and even in sign. Thus, the relative strengths and signs of \( V_{1,2,3} \) can be varied by changing the strength of the Zeemann splitting together with the detuning of the OFR laser. By contrast, in a standard magnetic FR, \( U_{-1} = U_{+1} \). In our case, breaking the symmetry between \( U_{-1} \) and \( U_{+1} \) leads to the orbital-changing term \( V_3 \). Physically, it allows \( (p_x \text{ or } p_y) \) particles to move on the two-dimensional plane, instead of along a chain only. Since it explicitly breaks time-reversal symmetry (TRS), we can expect it to lead to novel phases reflecting that intriguing property.

Hamiltonian \( 1 \) generalizes the models of Refs. \( 17, 22 \). For \( V_1 = V_2 \), and \( V_3 = 0 \), it reduces to the SU(3) Hubbard model. One can visualize \( p \)-band fermions as particles carrying a color index representing the \( p_x, p_y \), and \( p_z \) orbital states. Then, Hamiltonian \( 1 \) describes a three-color fermion model with color-dependent interaction, a novel color-changing term \( V_3 \), and spatially anisotropic and color-dependent tunneling. We will show below that this model has a rich phase diagram with novel phases. Here, we focus on the strong-coupling limit for \( p \)-band filling 1/3, and determine the orbital order using a Gutzwiller mean-field ansatz.

In the strong-coupling limit, \(|t_1| \ll V_1, |t_2| \ll V_2 - V_3, \text{ and } |t_3| \ll V_2 + V_3 \), double occupancies of the same site is suppressed. At 1/3 filling of the \( p \)-band, there is on average one \( p \)-band particle per site, and density fluctuations are frozen. Virtual hopping induces exchange interactions between nearest-neighbor orbitals (see Fig. \( 1 \)). The situation bears some resemblance to the emergence of magnetic models, such as the Heisenberg model, in the strong-coupling limit of the Hubbard model. The difference here is that three orbital (instead of two spin) states are involved. Since \( |t_1| \ll |t_2| \), perpendicular tunneling \( t_\perp \) can safely be neglected \( 19 \), and, for brevity, we write \( t = t_\parallel \). Treating the tunneling \( t \) in \( 1 \) as a perturbation and following standard second-order perturbation theory, we obtain the effective Hamiltonian for 1/3 filling:

\[
H_{\text{eff}} = -\sum_i \left[ \sum_{\mu=x,y,z} \sum_{\delta=\pm x} J_\mu n_{\mu,i} (1 - n_{\mu,i+\delta}) + \sum_{\mu=x,y} \sum_{\delta=\pm x} (J_2 - J_1) n_{\mu,i} n_{z,i+\delta} - \sum_{\delta=\pm x} J_3 (n_{x,i} c_{y,i} n_{z,i+\delta} + h.c.) \right], \tag{3}
\]

where we have used the constraint \( n_{x,i} + n_{y,i} + n_{z,i} = 1 \), and defined \( J_1 \equiv t_2/V_1 \), \( J_2 \equiv t_2^2/V_2 (V_2^2 - V_3^2) \), \( J_3 \equiv t_2^2 V_3/(V_2^2 - V_3^2) \), and \( J_z = J_3 = J_1 \). For \( V_3 = 0 \), \( V_1 = V_2 \), Eq. \( 3 \) reduces to \( J_3 n_{\mu,i} n_{\mu,i+\delta} \), a hallmark of the quantum 3-state Potts-like model \( 23 \).

To see which orbital order is favored, we first discuss the simple case of \( J_3 = 0 \). The first term of Eq. \( 3 \) always favors configurations where the orbitals at neighboring sites differ. (A) For \( J_1 > \text{max} (J_2,0) \), both the first and second terms favor an alternating pattern between \( p_x \) and \( p_y \)-particles in the \( xy \)-plane. (B) For \( J_2 > \text{max} (J_1,0) \), the favored configuration is an alternating pattern between \( p_z \) and \( \text{not-}p_z \). (C) For the (unstable case) \( J_1, J_2 < 0 \), the best configuration is a homogeneously filled lattice.

Certain aspects of Hamiltonian \( 3 \) become clearer when we rewrite it in terms of the generators of the SU(3) group. In terms of the Gell-Mann matrices \( \lambda^{(i)} \)}
and the so-called $F$-spin operators $Y = \frac{1}{\sqrt{3}} c_\mu^\dagger \lambda_\mu^{(8)} c_\nu$ and $T^{(\alpha)} = \frac{1}{2} c_\mu^\dagger \lambda_\mu^{(\alpha)} c_\nu$ ($\alpha = 1, 2, 3$), $H_{\text{eff}}$ becomes

$$H_{\text{eff}} = \frac{4}{3} \sum_i \left( (J_2 - J_1) Y_i - \frac{J_3}{4} T_i^{(2)} \right) + 2 \sum_i \left[ \sum_{\delta = e_x, e_y} (J_1 T_i^{(3)} T_i^{(3)\dagger} + \frac{2 J_2 - J_1}{4} Y_i \delta + \frac{J_2}{2} T_i^{(3)} Y_i \delta + \frac{J_2}{2} T_i^{(3)\dagger} Y_i \delta + J_3 T_i^{(2)} Y_i \delta + J_3 T_i^{(2)} Y_i \delta) \right],$$

where we neglected constant terms. In the basis $(p_x, p_y, p_z)$, $Y$ and $T^{(3)}$ are diagonal, which means that terms such as $Y_i Y_j$, $Y_i T^{(3)}_i$, or $T^{(3)}_i T^{(3)\dagger}_i$ are Ising-like. The orbital-changing term $V_3$ leads to $T^{(2)} = \frac{1}{2} (T^{(+)} - T^{(-)})$, where $T^{(\pm)}$ are ladder operators of the $T$-spin. $T^{(3)}$ and $T^{(2)}$ do not commute, but both commute with $Y$. This means that one can replace $Y$ by its eigenvalues $-\frac{1}{2}$ (for $|p_z\rangle$) and $\frac{1}{2}$ (for $|p_x\rangle$ and $|p_y\rangle$), which gives some insight into the physics of Hamiltonian $H$. Assuming that the ground state is bipartite with respect to the eigenvalue of $Y$, there are three different cases: (A) at all sites the eigenvalue of $Y$ is $\frac{1}{2}$, (B) the eigenvalues $-\frac{1}{2}$ and $\frac{1}{2}$ alternate, and (C) all sites have eigenvalue $-\frac{2}{3}$. In the last case, there is one $|p_z\rangle$-particle per site, whereas there is no virtual tunneling, and the Hamiltonian vanishes. In the sectors A and B, it reads (neglecting constant terms)

$$H_{\text{eff}}^{(A)} = \frac{J_1}{2} \sum_i \sum_{\delta = e_x, e_y} \sigma_i^{(3)} \sigma_{i+\delta},$$

$$H_{\text{eff}}^{(B)} = -2 J_3 \sum_{i \in \Omega} \sigma_i^{(2)}.$$ 

Here, $\sigma$ denotes the usual Pauli matrices, which act on the subspace spanned by $|p_x\rangle$ and $|p_y\rangle$. Sector A is reduced to the Ising model on decoupled $xy$-planes, which favors an antiferromagnetic ground state. This is just the model found in the 2D-case treated in [19, 20]. In sector B, $\Omega$ denotes the partition where $Y$ has eigenvalue $\frac{1}{2}$. On these sites, $J_3$ acts as a magnetic field in the $y$-direction, lifting the degeneracy between $|p_x\rangle$ and $|p_y\rangle$ and leading to the ground state $(|p_z\rangle \pm i |p_y\rangle)/\sqrt{2}$ (for $J_3 \geq 0$).

Having obtained a qualitative picture of the expected phases, we now analyze the phase diagram of Hamiltonian $H[1]$ quantitatively. To this, we assume that correlations between sites are small so that the ground state can be approximated by a product over sites. To find the ground state of Hamiltonian $H[1]$, we employ the Gutzwiller variational wave function $|\Psi\rangle = \bigotimes_i (\cos \theta |p_{2z}\rangle + \sin \theta \cos \phi |p_y\rangle + \sin \theta \sin \phi |p_{2z}\rangle)$, which is a product over sites $i$, and minimize the energy of a cube with side length $L$ (up to $L = 8$) under periodic boundary conditions. Note, however, that close to phase transitions, where fluctuations become important, such a mean-field ansatz is not valid.

The energy per site for even $L$ is smaller than for odd $L$, showing that the ground state periodicity is indeed 2. In agreement with the qualitative picture above, we find three classes of ground states with different orbital order (summarized in Fig. 2): (A) For $J_1 > J_2 = |J_3|/2$ and $J_1 > 0$, we find an ‘antiferromagnetic phase’ similar to, e.g., the 2D-model of Ref. [19]: in each $xy$-plane, sites with $p_x$- and $p_y$-orbitals alternate (similar to the antiferromagnetic Néel state). Since $p_x$- and $p_y$-particles do not tunnel in the $z$-direction, the $xy$-planes are decoupled, and within our approximation (e.g., neglecting $t_{\perp}$), there is no long-range order in the $z$-direction. It is possible, however, that long-range order among the planes develops at low temperature for finite $t_{\perp}$. (B) For $J_1 < J_2 = |J_3|/2$ and $J_2 > -|J_3|/2$, the ground state shows axial orbital order. The state is bipartite with $|p_z\rangle$ on one sublattice and $(|p_x\rangle \pm i |p_y\rangle)/\sqrt{2}$ (for $J_3 \geq 0$, respectively) on the other sublattice (right-hand panel of Fig. 2). The degeneracy between $|p_x\rangle$ and $|p_y\rangle$ is lifted by a finite $J_3$. The state $(|p_x\rangle \pm i |p_y\rangle)/\sqrt{2}$ has finite angular momentum, this novel phase breaks TRS. (C) For $J_1 < 0$ and $J_2 < -|J_3|/2$ Pauli exclusion prohibits all tunneling $t_{\parallel}$ (by filling $\alpha \beta$-planes ($\alpha \beta = xy, xz, yz$) uniformly with $p_x$ or $p_y$). This state is unstable, however, because it cannot fulfill the strong-coupling requirements [2]. Interestingly, phases A and C preserve TRS, although $V_3$ in Hamiltonian $H[1]$ breaks it explicitly.

Experimentally, the different phases can, e.g., be distinguished by measuring the density distribution after a time of flight $t_{\text{td}}$. This relates to the in-trap momentum distribution via $\langle n(r) \rangle_{t_{\text{td}}} = \ldots$
observed by the density distribution of the OFR. The system can be realized in a variety of systems with spinless fermions in the $p$-band of a cubic lattice with interaction controlled by an OFR. The system can be realized with current technology. The model Hamiltonian can be expressed elegantly by Gell-Mann matrices. We analyzed the orbital order in the strong-coupling limit at $p$-band filling $1/3$ using a Gutzwiller-type ansatz. Besides a phase where all tunneling is blocked and an antiferroorbital phase where $p_x$- and $p_y$-orbitals alternate, we found a novel phase with axial orbital order which not only breaks translational symmetry but also has macroscopic orbital angular momentum. We expect our results to stimulate future work on this subject. For example, it is interesting to investigate how quantum fluctuations affect the phase diagram: they might distort it or even lead to disordered 'orbital liquid' states. Fluctuations are also expected to lift the degeneracy between $p_x$- and $p_y$ orbitals at $J_3 = 0$, and possibly lead to spontaneous orbital liquid states. Fluctuations may have interesting topological properties. For example, at an interface of two domains with $p_x + ip_y$ and $p_x - ip_y$ order, chiral zero mode fermions may arise. Finally, other lattices and the limit of small interactions, where related models show non-trivial color-superfluidity [17, 18, 21], are also interesting.

This work is supported in part by NSF Grant PHY05-51164. P. H. and M. L. acknowledge support by the Caixa Manresa, Spanish MICINN (FIS2008-00784 and Consolidator QOIT), EU Projects AQUITE and NAMEQUAM, and ERC Grant QUAGATUA. E. Z. is supported by NIST Grant 70NANB7H6138 Am 001. W. V. L. is supported by ARO (W911NF-11-1-0230) and DARPA-OLE (ARO W911NF-07-1-0464). K. G. and I. H. D. are supported by NSF Grant PHY-0903953.
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[23] Orbital order in a simpler model without OFR, and its relation to the Potts model were discussed in the unpublished work of arXiv:0801.0888v1 by C. Wu.
[24] In principle, more complex (i.e., non-bipartite) partitions are possible, but the numerical mean-field analysis (see below) shows that these are the only relevant ones.
[25] Further, we checked that for even $L$ the occurring phases do not depend on $L$.
[26] The derivation of (4) neglected repulsive off-site interactions $n_{\mu,i}n_{\mu,i+\delta}$, which for $p$-band fermions might be important compared to the exchange couplings $J$. However, the alternating occupations in the (physically relevant) phases A and B also minimize possible energy contributions from off-site repulsions. Hence, neglecting these is justified a posteriori.
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