

Fermions in optical lattices near a Feshbach resonance: From band insulator to Mott insulator

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We study a model of an equal mixture of two species of fermions in a deep optical lattice at a filling of two fermions per site. At weak interspecies interaction, the system is a band insulator. When the interspecies interaction is tuned via a Feshbach resonance to be larger than an energy related to the energy separation of the first and second Bloch bands, atoms populate equally the two Bloch bands. With weak tunneling between sites of the optical lattice, the system becomes a Mott insulator with the low-energy effective Hamiltonian of a spin-1 Heisenberg antiferromagnet, because of a Hund's-rule-like coupling between the two bands. We discuss experimental signatures of these two types of insulators.

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The controllability and the capability to continuously tune parameters has provided unprecedented opportunities to study strong-correlation physics in trapped ultracold-atom systems. Thus, Greiner *et al.* [1] observed the quantum phase transition from a superfluid to a Mott insulator for bosons trapped in an optical lattice, by suppressing tunneling between sites of the lattice. Recently, there has been much experimental progress in studying fermionic superfluidity in the BCS to Bose-Einstein condensate crossover regime [2] whereby the scattering length between two species of fermions is continuously tuned through a Feshbach resonance [3].

In an optical lattice, the hopping matrix element t and the on-site interaction strength U both depend essentially on the amplitude V_0 of the laser beams that define the optical lattice [4]. But by adding an appropriate magnetic field to sweep through a Feshbach resonance, a larger range of U vs t can be accessed experimentally. Very recently, Köhl *et al.* [5] have exploited this to study two hyperfine states of fermionic ^{40}K (about a 50:50 mixture) loaded into a three-dimensional (3D) optical lattice. Initially, far from the Feshbach resonance (i.e., no interaction), the lattice is loaded with two fermions per site (one for each spin state) into the lowest Bloch band, with weak tunneling between sites. Hence the system is a band insulator. Now turning up the magnetic field toward the interspecies Feshbach resonance causes U to increase to bigger than the interband energy; hence atoms are measured being kicked into upper Bloch bands. The key question [6] is this: What happens to the band insulator as the Feshbach resonance is approached?

For atoms with Feshbach-resonance-enhanced interactions, Diener and Ho [6] have shown in the single-site problem and Katzgraber *et al.* [7] in the full lattice problem that there can be a window of magnetic field where essentially two Bloch bands are occupied: the harmonic oscillator ground state [000], together with the [001] band for an anisotropic lattice (as in the experiment of [5]). At or very near the Feshbach resonance itself, more bands may be occupied.

Thus, motivated by the experiment of [5], we study in this paper a simple model of spin-1/2 fermions in an optical lattice at a filling of two fermions per site, with equal mix of the two spin species, and where two Bloch bands are active, as a function of U :

$$H = \sum_{\alpha,\beta} \sum_{\sigma,i} -t_{\alpha\beta} c_{i+1\sigma\alpha}^\dagger c_{i\sigma\beta} + \text{H.c.} - \sum_{\alpha i \sigma} \mu_\alpha n_{i\sigma\alpha} + \sum_{\alpha i} U_{\alpha\alpha} n_{i\uparrow\alpha} n_{i\downarrow\alpha} + \sum_{\alpha \neq \beta, i} U_{\alpha\beta} [n_{i\uparrow\alpha} n_{i\downarrow\beta} - S_{i\alpha}^+ S_{i\beta}^- + \Delta_{i\alpha}^\dagger \Delta_{i\beta}], \quad (1)$$

where the band index $\alpha, \beta = 0, 1$ for the [000] and [001] bands, the “spin” [8] index $\sigma = \uparrow, \downarrow$, and the site index is i . $n_{i\sigma\alpha} = c_{i\sigma\alpha}^\dagger c_{i\sigma\alpha}$, $S_{i\alpha}^+ = c_{i\uparrow\alpha}^\dagger c_{i\downarrow\alpha}$, and $\Delta_{i\beta} = c_{i\downarrow\beta} c_{i\uparrow\beta}$. The chemical potential difference $\mu_0 - \mu_1 = \omega_0$ is the difference in energy between the two bands. For simplicity, we here consider only a 1D system. This is achieved in the experiments of [9] by setting the laser amplitudes $V_{0x} \ll V_{0y} = V_{0z}$, thereby creating an uncoupled set of 1D tubes [9], where excitations transverse to the tube axis are completely frozen. For higher dimensions, because of the spatial anisotropy of the [001] orbital, the hopping matrix element $t_{\alpha\beta}$ acquires spatial anisotropy also which complicates analysis [10,11].

This Hamiltonian has a similar form to those in solid state systems when multiple orbitals are active in, e.g., transition metal oxides [14]: the $-S^+ S^-$ term gives rise to Hund's rule in atomic physics, which favors spin alignment between different orbitals. The difference here in the optical lattice is that the atomic interactions are contact interactions, not the long-range Coulomb interactions for electrons in solids. Hence, the Hund's rule term is of the same order of magnitude as the on-site repulsion term, unlike in solids. Also unlike in solids, experimental preparation [5] dictates that the number of fermions for *each* spin species is conserved separately.

In this paper, we study this model Eq. (1) at weak intersite tunneling and at zero temperature. We show that when the Feshbach-tunable interactions are weak compared to the interband energy ω_0 , a “spin” singlet [8] of two fermions resides in each lattice well in the lowest Bloch band to form a band insulator. When the interactions are strong relative to ω_0 , the two fermions at each site reside in different bands with aligned spin, forming an effective spin 1. This effective spin 1 alternates in sign between neighboring sites to take advantage of second-order virtual hopping of the fermions, thereby forming a spin-1 Heisenberg antiferromagnet

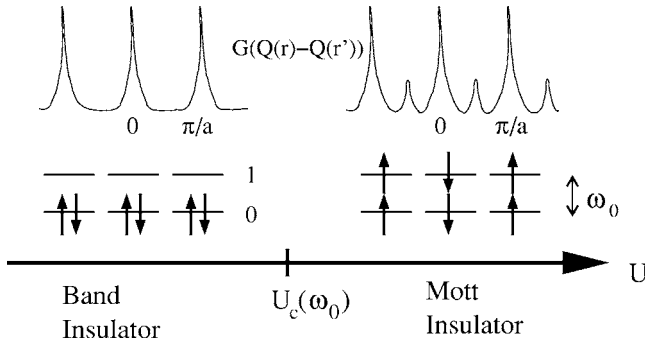


FIG. 1. Schematic phase diagram. The middle row shows the dominant spatial structure of the two species (spin) of fermions in orbitals 0 and 1; the top row shows the schematic correlation function $G(r, r')$ which may be measured in noise correlation experiments: the Mott insulator has extra peaks due to doubling of the real-space unit cell.

(see Fig. 1). This is a correlated (Mott) insulator state as each band is only half filled, and is reminiscent of the charge-transfer insulator in transition-metal compounds [12] and excitonic insulators [13].

The use of Feshbach resonance to populate higher Bloch bands of optical lattices promises to open up much interesting orbital physics that may go beyond those models studied in the context of transition-metal oxides [14]. For example, in 2D and 3D, there can be orbital spatial ordering in a lattice with a single species of bosons [10]. Duan [15] has also studied the effect of Feshbach resonance on fermions in optical lattices, but as that study was in a different regime, he found effective models with spin-1/2 antiferromagnetic correlations.

The microscopic 1D Hamiltonian is

$$\begin{aligned}
 H = & \sum_{\sigma} \int_0^L dx \frac{1}{2M} [\partial_x \psi_{\sigma}^{\dagger}(x) \partial_x \psi_{\sigma}(x)] \\
 & + \sum_{\sigma} \int_0^L dx (V_{0x} \sin^2 kx - \mu) \psi_{\sigma}^{\dagger}(x) \psi_{\sigma}(x) \\
 & + \frac{g}{2} \int_0^L dx \psi_{\uparrow}^{\dagger}(x) \psi_{\downarrow}^{\dagger}(x) \psi_{\downarrow}(x) \psi_{\uparrow}(x). \quad (2)
 \end{aligned}$$

Since we are interested in the regime where at most two Bloch bands are occupied (roughly, $U < 2\omega_0$), we expand the operator $\psi_{\sigma}(x)$ in Wannier functions, $\psi_{\sigma}(x) = \sum_{\alpha=0,1} w_{i\alpha}(x) c_{i\sigma\alpha}$, where for a deep optical lattice, we approximate the Wannier functions by *local* harmonic oscillator orbitals. I shall consider band 0 to be the ground state $w_{i0}(x) = \frac{1}{(\pi a_0^2)^{1/4}} \exp\left(-\frac{(x-x_i)^2}{2a_0^2}\right)$, and band 1 to be the first excited state $w_{i1}(x) = \frac{(-1)^i \sqrt{2(x-x_i)}}{(\pi a_0^2)^{1/4} a_0} \exp\left(-\frac{(x-x_i)^2}{2a_0^2}\right)$. Note that these functions, unlike Wannier functions, are not orthogonal for different bands with respect to the hopping; hence there can be band-changing hopping with $t_{01} = t_{10}$. In fact, in general for band 1 to have a higher energy, $|t_{00}| < |t_{01}| < |t_{11}|$.

Then substituting the approximate Wannier functions into

Eq. (2) gives the Hamiltonian of Eq. (1), with the parameters $U_{00} = c_{00}U$, $U_{01} = c_{01}U$, $U_{11} = c_{11}U$, $U = \frac{a_s k (4\bar{V})^{3/4}}{\sqrt{\pi} E_r}$, $\bar{V} = (V_{0x} V_{0y} V_{0z})^{1/3}$. (We are giving the values for the actual 3D situation wherein the 1D tubes are embedded, i.e., $V_{0x} \ll V_{0y} = V_{0z}$ [9]). a_s is the Feshbach-resonance-enhanced effective scattering length between the species, which can be tuned by the magnetic field [16]. In general a_s will depend on the energy of the two scattering particles, and is renormalized from the free-space value by strong transverse confinement and the Feshbach resonance. In absence of calculations, we have left as parameters $c_{\alpha\beta}$ to denote this band dependence. As a crude guide, treating a_s as energy independent, $c_{00} = 1$, $c_{01} = 1/2$, $c_{11} = 3/4$, and a_s refers then to some average value, but with Feshbach and transverse confinement renormalization. We only consider the situation where the broad Feshbach resonance is approached from the side where the scattering length is positive, with few if any molecules formed. Hence sweeping the magnetic field toward the Feshbach resonance effectively makes the couplings $U_{\alpha\beta} \propto g = 4\pi a_s / M > 0$ grow from $U_{\alpha\beta} \ll \omega_0$ to $U_{\alpha\beta} \gtrsim \omega_0$. We have approximated the interband energy ω_0 to be just the harmonic oscillator energy in the x direction, $\omega_0 \approx \sqrt{4V_{0x} E_r}$, with $E_r = k^2 / 2M$ the recoil energy for the optical lattice, $k = 2\pi / \lambda$ where λ is the laser wavelength, with the lattice spacing $a = \lambda / 2$.

Köhl *et al.*'s experiment [5] is in the strong-coupling limit, so we focus on $t_{\alpha\beta} \ll \omega_0, U_{\alpha\beta}$. Thus, first diagonalize the Hamiltonian Eq. (1) with $t_{\alpha\beta} = 0$ to get the local spectrum with two fermions (one of each spin) per site:

$$E_+^{(t)} = -2\mu_0 + \omega_0, \quad |t+\rangle = \frac{1}{\sqrt{2}}(|\uparrow;\downarrow\rangle + |\downarrow;\uparrow\rangle),$$

$$E_-^{(t)} = -2\mu_0 + \omega_0 + 2U_{01}, \quad |t-\rangle = \frac{1}{\sqrt{2}}(|\uparrow;\downarrow\rangle - |\downarrow;\uparrow\rangle),$$

$$\begin{aligned}
 E_{\pm}^{(s)} = & -2\mu_0 + \omega_0 + \frac{U_{00} + U_{11}}{2} \\
 & \mp \left[\left(\frac{U_{11} - U_{00}}{2} + \omega_0 \right)^2 + U_{01}^2 \right]^{1/2},
 \end{aligned}$$

$$|s+\rangle = a_1 |\uparrow\downarrow; 0\rangle + a_2 |0; \uparrow\downarrow\rangle,$$

$$|s-\rangle = a_2 |\uparrow\downarrow; 0\rangle - a_1 |0; \uparrow\downarrow\rangle. \quad (3)$$

The notation for the eigenstates is that the leftmost slot is for band 0, separated by a semi-colon from the band 1 slot. (We have dropped the site index on the eigenstates.) a_1, a_2 are functions of $U_{\alpha\beta}$ and ω_0 with $a_1^2 + a_2^2 = 1$. In Fig. 2, we plot the probability of a singlet in band 0 or band 1, using $c_{00} = 1$, $c_{01} = 1/2$, $c_{11} = 3/4$.

Since $U_{\alpha\beta} > 0$, the lowest energy is $E_+^{(s)}$ for $U_{\alpha\beta} < U_{\alpha\beta}^c$ or $E_+^{(t)}$ when $U_{\alpha\beta} > U_{\alpha\beta}^c$. The two levels cross at $U_{\alpha\beta}^c(\omega_0)$ given by the implicit equation $(U_{01}^c)^2 = (U_{00}^c - \omega_0)(U_{11}^c + \omega_0)$. Note that there is only one transition, since all the $U_{\alpha\beta} \propto U$. Right at the transition, the parameters a_1, a_2 have the simple form $a_1 = -\left(\frac{U_{11}^c + \omega_0}{U_{00}^c + U_{11}^c}\right)^{1/2}$, $a_2 = \left(\frac{U_{00}^c - \omega_0}{U_{00}^c + U_{11}^c}\right)^{1/2}$. Thus, when $U_{\alpha\beta} < U_{\alpha\beta}^c$, at

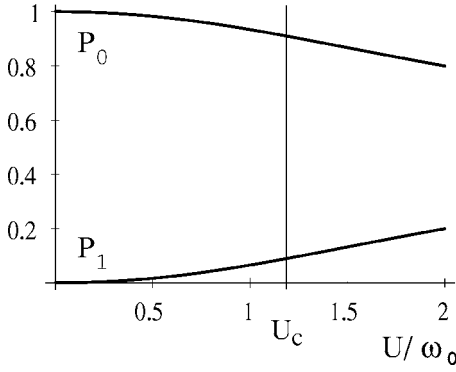


FIG. 2. Probability of a singlet in band 0 (P_0 , upper curve) or band 1 (P_1 , lower curve) as a function of U/ω_0 , for the eigenstate $|s+\rangle$. The vertical line shows the location of U_c . Note that $|s+\rangle$ is the ground state only for $U < U_c$, and for $U \geq 2\omega_0$, higher bands start to be occupied.

each site, the ground state is $|s+\rangle$ with a singlet in band 0 mixed in with a bit of the singlet in band 1, while for $U_{\alpha\beta} > U_{\alpha\beta}^c$, the ground state is a spin triplet with one fermion in each band, $|0\rangle \equiv |t+\rangle$. Note that this triplet is degenerate with the other two members of the spin triplets: $|U\rangle = |\uparrow; \uparrow\rangle$, $|D\rangle = |\downarrow; \downarrow\rangle$. In Köhl *et al.*'s experiment, when the interspecies interaction is gradually turned up, the states $|U\rangle, |D\rangle$ cannot be reached at any sites if there is no hopping at all between the sites.

When the hopping is switched on, the effective low-energy Hamiltonian can be derived using the usual strong-coupling expansion to $O(t^2/U)$, where intermediate states have a site and its neighbor having three and one fermions, respectively. We find [11] that for $U_{\alpha\beta} < U_{\alpha\beta}^c$, the system is still a band insulator, while for $U_{\alpha\beta} > U_{\alpha\beta}^c$, the system is now a Mott (correlated) insulator, with interesting spin dynamics which is that of the spin-1 Heisenberg antiferromagnet:

$$H_{U>U_c} = J \sum_i (\vec{S}_i \vec{S}_{i+1} - 1), \quad (4)$$

$$J = \frac{t_{00}^2}{U_{00} + U_{01}} + \frac{t_{11}^2}{U_{11} + U_{01}} + t_{01}^2 \left(\frac{1}{U_{00} + U_{01} - \omega_0} + \frac{1}{U_{11} + U_{01} + \omega_0} \right) \quad (5)$$

where \vec{S} is a spin-1 operator. Spin 1 is involved because of the spin degeneracy of the triplet states. Unlike the 1D spin-1/2 antiferromagnet which has no spin gap, the spin-1 case in 1D has a gap $\approx 0.41J$ (the Haldane gap [19,20]).

At $U_{\alpha\beta} = U_{\alpha\beta}^c$, four states (the spin-1 triplet and $|t+\rangle$) are now degenerate locally. The effective Hamiltonian at the transition point corresponds to a spin ladder, where each leg is a spin-1/2 Heisenberg antiferromagnet, with exchange couplings between the sites on a rung of the ladder (i.e., $\vec{S}_i^{(\alpha)} \vec{S}_i^{(\alpha)}$, where α is now the ladder leg index), but also diagonally (i.e., $\vec{S}_i^{(1)} \vec{S}_{i+1}^{(2)}$, where 1,2 label the two legs). Full details will be published elsewhere [11]. We just point out

here that generically such spin ladders have a spin gap [17,18]. Hence it is likely that over the whole phase diagram as a function of U , the spin gap persists.

So far, we have focused on the large- U limit and found only insulators. Clearly, when $t_{\alpha\beta} \gg \omega_0, U_{\alpha\beta}$, the system will be a metal. Thus in the whole phase diagram there should be metal-insulator transitions together with some multicritical point. Work is in progress to explore this rich phase diagram.

Both the band insulator and the Mott insulator have an energy gap to “charge” excitations, and interestingly, also for spin excitations. However, for this band to Mott insulator quantum phase transition, there are spin gaps (and also charge gaps) all the way from $U_{\alpha\beta} < U_{\alpha\beta}^c$ to $U_{\alpha\beta} > U_{\alpha\beta}^c$ (except perhaps right at the transition?), so a spin gap (as might be measured via two-photon Raman transitions [21,22]) does not qualitatively distinguish the band vs the Mott insulator. The smoking gun experiment would be to image the up spins populating one sublattice while the down spins populate the other.

But even without direct spin- and site-dependent imaging, current experimental probes such as noise correlation [23,24] from time-of-flight (TOF) imaging may distinguish between the band insulator and the Mott insulator. The 1D momentum distribution can be readily evaluated, assuming that deep in the insulator phases, charge fluctuations are frozen. Thus, for the band insulator phase where most weight is in the band 0, $n(Q_r) \sim \rho_0 |w_0(Q_r)|^2$, while for the Mott insulator, with one fermion in each band at each site, $n(Q_r) \sim \rho_0 (|w_0(Q_r)|^2 + |w_1(Q_r)|^2)/2$. $Q_r = Mr/t$ is the continuum momentum with r the imaging position relative to the initial distribution of cold atoms, and t is the time of flight. This change in the filling of the bands may have been observed in [5].

To probe the spin spatial structure, one has to go to the noise correlation in the TOF imaging, which measures $G(r, r') = \sum_{\sigma\sigma'} \langle n_{\sigma}(Q_r) n_{\sigma'}(Q_{r'}) \rangle - \langle n_{\sigma}(Q_r) \rangle \langle n_{\sigma'}(Q_{r'}) \rangle$ [23]. A straightforward generalization to the two-band case gives a number of terms that show differences between the two types of insulators, but the key signature comes from the static spin structure factor [23] part within $G(r, r')$. Because of the different spatial symmetry of the Wannier functions of the two bands, $G(r, r')$ does not directly probe the effective spin-1 correlations of the Mott insulator, but instead has information on individual band spin correlations:

$$G(r, r') \sim -2 \sum_{\alpha\beta} \sum_{nm} e^{i(Q_r - Q_{r'})(r_n - r_m)} \times w_{\alpha}^*(Q_r) w_{\beta}(Q_r) w_{\beta}^*(Q_{r'}) w_{\alpha}(Q_{r'}) \times \left\langle \vec{S}_{\alpha n} \vec{S}_{\beta m} - \frac{1}{4} n_{\alpha n} n_{\beta m} \right\rangle + \dots, \quad (6)$$

where $\vec{S}_{\alpha n}$ is a spin-1/2 operator of band α at site $r_n = na$. (The ellipsis refers to other terms without lattice periodicity mentioned above; we shall henceforth ignore them.) For the band insulator, since at each site there is a singlet in band 0, there is no spin-spin correlation contribution, and $G(r, r') \propto \frac{1}{2} |w_0(Q_r)|^2 |w_0(Q_{r'})|^2 \sum_G \delta(Q_r - Q_{r'} + G)$, where G is a reciprocal lattice vector (integer multiples of $2\pi/a$).

For the Mott insulator, assuming equal spin-spin correlations for the two bands and between bands,

$$G(r, r') \propto - \left[\frac{1}{2} \sum_G \delta(Q_r - Q_{r'} + G) + 2 \sum_G f \left(Q_r - Q_{r'} + \frac{\pi}{a} + G \right) \right] \times \sum_{\alpha\beta} w_{\alpha}^*(Q_r) w_{\beta}(Q_r) w_{\beta}^*(Q_{r'}) w_{\alpha}(Q_{r'}). \quad (7)$$

Thus, just as for the spin-1/2 Heisenberg antiferromagnet, a sharp (only relatively so in 1D) peak of form $f(Q)$ (see, e.g., [23]) occurs in between the Bragg peaks at G , thanks to the doubling of the unit cell in real space for the antiferromagnet (see Fig. 1). The appearance of this extra peak constitutes proof of the spin structure, while the existence of a spin gap distinguishes between a spin-1 and a spin-1/2 antiferromagnet.

We have assumed so far that the system is homogeneous and large. In experiments [5], the system consists of around $\sim 10^5$ fermions in a few thousand tubes, and the overall trapping potential leads to inhomogeneities in occupation per site across the tube. This inhomogeneity can lead to phase coexistence [25] of a Mott insulator surrounded by a shell of superfluidity for the bosonic Hubbard model. Nevertheless, the bosonic Mott insulator has been observed [1,24], and we expect the same to be possible for the fermionic model here, as long as there is a large enough central region with commensurate filling of two fermions per site. Also, in the experiment of [5], the number of spin-up fermions equals the down ones up to a few percent, and the spin-1 antiferromagnetic structure described above should persist in the Mott phase.

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