

Mott-insulator phases of spin-3/2 fermions in the presence of quadratic Zeeman coupling

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We study the influence of the quadratic Zeeman effect in the Mott-insulator phases of hard-core spin-3/2 fermions. We show that contrary to spinor bosons, any quadratic Zeeman coupling preserves a $SU(2) \otimes SU(2)$ symmetry, leading for large-enough quadratic Zeeman coupling to an isotropic pseudo-spin-1/2 Heisenberg antiferromagnet. Depending on the scattering lengths, on 1D lattices the quadratic Zeeman coupling can induce either a Kosterlitz-Thouless transition between a gapped dimerized spin-3/2 phase and a gapless pseudo-spin-1/2 antiferromagnet, or a commensurate-incommensurate transition from a gapless spin-liquid into the pseudo-spin-1/2 antiferromagnet. Similar arguments allow to foresee corresponding transitions on ladder type and square lattices. We analyze various observables which should reveal in experiments these phases.

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Ultra-cold gases in optical lattices constitute an extraordinary tool for the analysis of strongly-correlated gases under extremely well-controlled conditions [1, 2], as highlighted by the observation of the superfluid to Mott-insulator (MI) transition in ultra-cold bosons [3], recently followed by the realization of the metal to MI transition in two-component fermions [4, 5]. Due to superexchange, the MI phase of spin-1/2 fermions is expected to acquire a magnetic Néel (antiferromagnetic) ordering, whose observation is the goal of active on-going efforts [6].

Optical traps permit the simultaneous trapping of various Zeeman sublevels, allowing for multi-component (spinor) gases. Spinor bosons have attracted a large interest due to their rich ground-state physics and spinor dynamics [7]. Recently, spinor fermions are also attracting a rapidly-growing attention, motivated by experiments on BEC-BCS crossover in two-component fermions [2] and the availability of multi-component fermions, including three-component Li gases [8], four-component ^{40}K [9], spin-3/2 fermions as ^{135}Ba and ^{137}Ba [11], and Fermi-degenerate Yb [10]. Multi-component fermions present a wealth of novel phases. Pseudo-spin-1 fermions [12] allow for color superfluidity and trions, whereas spin-3/2 gases are even richer [13–16], including quartets. Ultra-cold Yb opens the fascinating possibility of $SU(6)$ -symmetric spin-5/2 gases [17].

A rich physics is also expected for repulsive spin-3/2 fermions [14, 15], which in quarter filling may undergo a MI transition. Whereas for spin-1/2 a Néel phase is expected, the MI in spin-3/2 presents a richer magnetic structure given by a gapless spin-liquid or a gapped dimerized phase, depending on the interatomic interactions. Contrary to the spin-1/2 case, where spin-changing collisions are absent and the quadratic Zeeman effect (QZE) is irrelevant, the QZE is crucial for higher-spins, as shown in spinor condensates [7]. However, in spite of its experimental relevance, the QZE has been typically ignored in the analysis of the magnetic properties.

In this Letter, we explore, for the first time to our

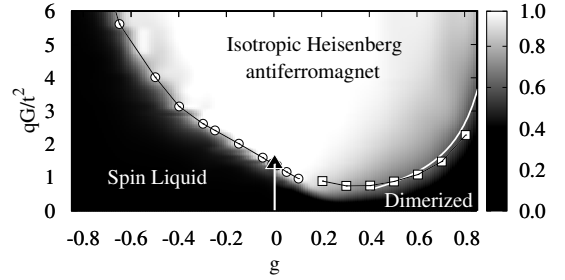


FIG. 1: Phase diagram for spin-3/2 fermions with QZE. We depict the chirality τ (density plot), the singlet-triplet crossing in the excitation spectrum (squares), the jump of the exponent γ to -1 (circles), the critical q_c expected from two-band theory (triangle), and the $J_2/J = 0.25$ line resulting from a strong-coupling analysis (white curve). See text.

knowledge, the role of the QZE in the magnetism of spin-3/2 MI phases. We show that contrary to spinor bosons [18], any QZE preserves a $SU(2) \otimes SU(2)$ symmetry which results at large QZE in a pseudo-spin-1/2 isotropic Heisenberg antiferromagnet (iHAF). Depending on the scattering lengths, our results suggest for growing QZE a Kosterlitz-Thouless (KT) phase transition (PT) from a gapped dimerized spin-3/2 phase into the iHAF, or a commensurate-incommensurate (C-IC) PT between a gapless spin-liquid again into the iHAF. We analyze in detail observables which may characterize the phases (Fig. 1) and PTs in future experiments [19].

We consider a balanced mixture of spin-3/2 fermions in a 1D lattice [20] with $N_m = N_{-m}$ ($N_m =$ number of fermions with spin projection m), such that the magnetization $\mathcal{M} \equiv \sum_m m N_m = 0$. For a deep lattice and low filling (single-band regime) the system Hamiltonian is

$$\hat{H} = -t \sum_{m,i} \left[\hat{\psi}_{m,j}^\dagger \hat{\psi}_{m,j+1} + \text{H.c.} \right] - q \sum_{m,j} m^2 \hat{n}_{m,j} + g_0 \sum_i P_{00,i}^\dagger P_{00,i} + g_2 \sum_{i,m_F} P_{2m_F,i}^\dagger P_{2m_F,i}, \quad (1)$$

where $\hat{\psi}_{m,j}$ annihilate fermions with spin m at site j , $F_{Fm_F,i}^\dagger = \sum_{m_1,m_2} \langle F, m_F | m_1, m_2 \rangle \psi_{m_1,i}^\dagger \psi_{m_2,i}^\dagger$, with $\langle F, m_F | m_1, m_2 \rangle$ the Clebsch-Gordan coefficients, and $\hat{n}_{m,j} = \psi_{m,j}^\dagger \psi_{m,j}$. t is the hopping rate between adjacent sites, and $g_{0,2} = 4\pi\hbar^2 a_{0,2}/M$ characterize the s -wave channels with total spin 0 and 2 (the only available due to symmetry), with $a_{0,2}$ the scattering lengths and M the atomic mass. Although typically a_0 and a_2 are similar, their values may be varied by means of microwave dressing [21] or optical Feshbach resonances [22]. Below we use $G = (g_0 + g_2)/2$, and $g = (g_2 - g_0)/(g_2 + g_0)$. The interactions preserve \mathcal{M} and hence the linear Zeeman effect induced by a magnetic field does not play any role for a fixed \mathcal{M} . However spin-changing collisions (which re-distribute the populations of the different components while preserving \mathcal{M}) are crucial. Finally, the QZE, characterized by the externally controllable (by means of a magnetic field or microwave or optical dressing) constant q , is crucial in spinor gases, and plays a key role below.

For large-enough interactions, $G \gg t$, we may consider the hard-core case, with maximally one fermion per site. For a chemical potential μ larger than a critical $\mu_c(t)$ the system enters into the MI regime with one fermion per site. We focus below in the magnetic properties of these MI phases. Within the MI regime we perform perturbation theory obtaining an effective Hubbard Hamiltonian with super-exchange interactions, which for two adjacent sites $\{1, 2\}$ is of the form $\hat{H}_{12} = \hat{H}_0 + \hat{H}_{sc}$, where

$$\begin{aligned} \hat{H}_0 &= - \sum_m qm^2 (\hat{n}_{m,1} + \hat{n}_{m,2}) \\ &+ c_2 \sum_{|m| \neq |m'|} \left(\hat{n}_{m,1} \hat{n}_{m',2} - \hat{\psi}_{m,1}^\dagger \hat{\psi}_{m',2}^\dagger \hat{\psi}_{m,2} \hat{\psi}_{m',1} \right) \\ &+ \sum_{|m|=1/2}^{3/2} c_{|m|} \left(\hat{n}_{m,1} \hat{n}_{-m,2} - \hat{\psi}_{m,1}^\dagger \hat{\psi}_{-m,2}^\dagger \hat{\psi}_{m,2} \hat{\psi}_{-m,1} \right) \end{aligned} \quad (2)$$

contains self-energies and effective hoppings without spin-changing, whereas a simultaneous hopping and spin-changing is given by $\hat{H}_{sc} = c_{sc} (\hat{B}_{1/2}^\dagger \hat{B}_{3/2} + \text{H.c.})$, with $\hat{B}_m = \hat{\psi}_{m,2} \hat{\psi}_{-m,1} - \hat{\psi}_{-m,2} \hat{\psi}_{m,1}$. We introduce above:

$$c_{3/2} \equiv -2t^2 \left(\frac{\cos^2 \phi}{9q/2 + \lambda_+} + \frac{\sin^2 \phi}{9q/2 + \lambda_-} \right), \quad (3)$$

$$c_{1/2} \equiv -2t^2 \left(\frac{\cos^2 \phi}{q/2 + \lambda_-} + \frac{\sin^2 \phi}{q/2 + \lambda_+} \right), \quad (4)$$

$$c_{sc} \equiv t^2 \sin 2\phi \sum_{\beta=\pm} \eta_\beta \frac{5q/2 + \lambda_\beta}{\prod_{\bar{m}=1/2}^{3/2} (2q\bar{m}^2 + \lambda_\beta)}, \quad (5)$$

with $\eta_\pm = \pm 1$, $\lambda_\pm \equiv G - 5q/2 \pm [4q^2 + g^2G^2]^{1/2}$, and $\tan \phi = ([4q^2 + g^2G^2]^{1/2} + 2q)/gG$.

Due to the spin-changing collisions, the single-site two-particle eigenstates with zero magnetization are not states with spins m and $-m$ ($|m, -m\rangle$), but the linear

combinations $|+\rangle = \cos \phi | -3/2, 3/2 \rangle + \sin \phi | -1/2, 1/2 \rangle$ and $|-\rangle = -\sin \phi | -3/2, 3/2 \rangle + \cos \phi | -1/2, 1/2 \rangle$ (with respective eigenenergies λ_\pm). This mixing leads to \hat{H}_{sc} and the non-trivial q and g dependence of $c_{3/2}$, $c_{1/2}$, and c_{sc} . Note that $c_{3/2}$, $c_{1/2}$, c_{sc} may diverge at specific values for which spin-changing collisions and QZE enter in resonance. Below we consider only non-resonant situations for which the hard-core formalism remains valid.

For $q = 0$ the ground-state of $H = \sum_i H_{i,i+1}$ only depends on g [14, 15]. For $-1 < g \leq 0$ the ground-state is a gapless spin liquid phase (with 3 gapless spin-modes). This phase includes the exactly solvable $SU(4)$ line ($g = 0$, i.e. $g_0 = g_2$) [23]. For $0 < g < 1$ the ground-state is a dimerized (spin-Peierls) phase which exhibits a spin gap and finite long-range dimer-dimer correlations $\lim_{n \rightarrow \infty} \langle D_i D_{i+n} \rangle = f_0$, with $\hat{D}_i = (-1)^i \hat{\mathbf{S}}_i (\hat{\mathbf{S}}_{i-1} + \hat{\mathbf{S}}_{i+1})$, with $\hat{\mathbf{S}}$ the spin-3/2 operators. At $g = 0$ the system undergoes a KT-like transition between both phases.

The $\pm 1/2$ and $\pm 3/2$ manifolds are just linked by \hat{H}_{sc} . Hence, at large-enough $q > 0$, when $\epsilon \equiv c_{sc}/(c_{1/2} - c_{3/2} - 2q) \ll 1$, the $\pm 3/2$ manifold is favored, and the system acquires a pseudo-spin-1/2 character. Below we restrict to $q > 0$, but similar reasonings apply to $q < 0$, for which the $\pm 1/2$ manifold is favored. Projecting onto the $\pm 3/2$ manifold and up to second order in $\epsilon > 0$, the Hamiltonian reduces to an isotropic Heisenberg form, $\hat{H}_{12} \simeq J \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$, where $J \equiv -2(c_{3/2} - 2\epsilon c_{sc})$ and \mathbf{S} denotes pseudo-spin-1/2 operators $\hat{S}_z \equiv (\hat{n}_{3/2} - \hat{n}_{-3/2})/2$, $\hat{S}_+ \equiv \hat{\psi}_{3/2}^\dagger \hat{\psi}_{-3/2}$ and $\hat{S}_- \equiv \hat{S}_+^\dagger$. Since $J > 0$ for all $g_0, g_2, q > 0$, the system reduces to an iHAF for large-enough q . This is true at any order in ϵ due to a hidden $SU(2)$ symmetry (see below). This must be compared to the case of spinor bosons [18], where virtual transitions between manifolds lead for large q to an anisotropic Heisenberg Hamiltonian, demanding a fine tuning of the microscopic constants to map the system to an iHAF.

Interestingly, spin-3/2 fermions, which show a hidden $SO(5)$ symmetry for $q = 0$ [13], retain at any q a $SU(2) \otimes SU(2)$ symmetry, generated by a direct product of two $SU(2)$ spin algebras operating in the $\pm 1/2$ and $\pm 3/2$ manifolds, respectively. The $SU(2)$ generators are $\hat{S}_z^\alpha = 1/2 \sum_i (\hat{n}_{\alpha,i} - \hat{n}_{-\alpha,i})$, $\hat{S}_\pm^\alpha = \sum_i \psi_{\alpha,i}^\dagger \psi_{-\alpha,i}$, with $\alpha = \{1/2, 3/2\}$. They belong to the $SO(5)$ algebra generating the $SO(5)$ symmetry for $q = 0$ and also commute separately with the QZE term. Note that this hidden $SU(2) \otimes SU(2)$ symmetry is related neither to the hard-core constraint nor to quarter filling, being rather a generic feature of $SO(5)$ fermions with QZE. This symmetry might be very helpful for future numerical simulations on four-component fermions in magnetic fields. For large q this symmetry results in the mentioned iHAF.

Growing q induces PTs between the $q = 0$ phases and the iHAF. We have obtained the ground state for various q and g by using the Density-Matrix Renormalization Group (DMRG) method of Ref. [24], with 36 sites, open

boundary conditions, and matrix dimension 20. The asymmetric phase diagram (Fig. 1), discussed in details below, is characterized by a re-entrant dimerized phase.

Case of $g > 0$. Bosonization shows that the dimerized phase is robust at small q , which induces a finite chirality $\tau = \frac{1}{2}[(N_{3/2} + N_{-3/2}) - (N_{1/2} + N_{-1/2})] \propto \tilde{q} \equiv qG/t^2$ (for $\tilde{q} \ll 1$). At large q bosonization is not appropriate, and one must instead descend from the iHAF decreasing q . Spin-changing processes lead to an AF frustrating next-nearest neighbour exchange J_2 ($\sim \tilde{q}^{-2}$) between pseudo-spins-1/2, resembling a frustrated spin-1/2 $J_1 - J_2$ AF chain, which presents a PT at $J_2/J_1 \simeq 0.25$ [25]. Hence a PT can be anticipated between the iHAF and the dimerized phase since when lowering \tilde{q} and increasing g the ratio J_2/J_1 increases. Fig. 1 shows the curve $J_2/J_1 = 0.25$ obtained from perturbation theory, which is in good agreement with the results discussed below.

A strong-coupling analysis is however not a reliable proof of the existence of an actual PT, and numerical calculations must be performed to confirm it. In a finite chain the two ground states of the dimerized phase (degenerate in the thermodynamic limit) split into a unique ground state and an excited one separated by an energy gap exponentially small in the system size. Thus, for finite chains the lowest excited state in the dimerized phase is unique (for $0 < q < q_{cr}$). In contrast, the lowest excited state above the Heisenberg ground state ($q > q_{cr}$) for a finite size chain is a degenerate triplet. If the PT is of KT type, as in a frustrated spin-1/2 $J_1 - J_2$ AF chain, a level crossing between the lowest excited singlet and triplet states should occur. Exact Lanczos diagonalization results, for up to 12 sites with periodic boundary conditions and performing finite size scaling, confirm indeed this crossing. The extrapolated q_{cr} lies in the region expected from the DMRG calculation of τ (grey region on the $g > 0$ side of Fig. 1). Although this certainly suggests a direct KT PT from the dimerized phase to the iHAF, for large $g > 0$, our size limitations are too severe for small $g \ll 1$, and there we cannot exclude the existence of intermediate phases [26]. Hence, the iHAF chain undergoes a dimerization transition. For decreasing q the dimerized phase of the pseudo-spin-1/2 chain adiabatically connects with the dimerized phase of spin-3/2 fermions, as they share similar properties.

Although beyond the scope of this Letter, a rich physics is also expected in ladder-like and square lattices, since $\mathcal{O}(\tilde{q}^{-2})$ terms induce frustrating diagonal ($J_x > 0$) and next-nearest neighbor ($J_2 = 0.5J_x$) exchanges. On ladders an Ising PT is expected from a rung-singlet phase to a columnar-dimer state with growing frustration [30], while on a square lattice the Néel state may undergo a PT into a columnar-dimer state [31] possibly via a second-order PT showing deconfined quantum criticality [32].

We are interested in the ground-state characterization at finite q for $g \neq 0$. The dimer phase is characterized by a finite f_0 and a singlet-triplet gap Δ in the magnetic

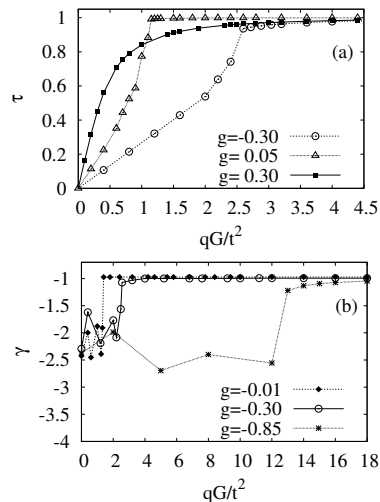


FIG. 2: Chirality τ (a) and exponent γ (b) as a function of q , for different values of g . DMRG results with 36 sites.

excitation spectrum [27]. Both f_0 and Δ vanish for the iHAF. We monitor as well spin-spin correlations, $\langle \hat{S}_z^i \cdot \hat{S}_z^j \rangle \propto |j - i|^\gamma$ [28], and the chirality τ , which ranges from 0 ($q = 0$) to 1 (pure iHAF). Fig. 2(a) shows DMRG results for τ . For weak $g > 0$ the system presents still a quasi-saturation of τ , which smoothly converges to 1 for large g . γ behaves similarly, jumping abruptly to -1 for small $g > 0$ (Fig. 1). f_0 and Δ evolve similarly.

Case of $g \leq 0$. In this case there is a PT between two gapless phases for increasing q . For $g = 0$ (no spin-changing collisions) the critical properties as a function of q resemble those of a two-band model [29], where atoms with $m = \pm 1/2$ ($\pm 3/2$) act as fermions at the lowest (second) band, and the QZE difference $2q$ resembles the band gap. For $\tilde{q} < \tilde{q}_0 \equiv 2 \ln 2 \simeq 1.386$ the magnetic order is suppressed due to “orbital” effects, and the system has three massless spinons. On the contrary for $\tilde{q} > \tilde{q}_0$ the “orbital” degeneracy is lifted, and the manifolds $\pm 1/2$ and $\pm 3/2$ completely decouple in the ground state. When this occurs, τ saturates to 1, and the system reduces, as mentioned above, to a pseudo-spin-1/2 iHAF with $J = 2t^2/G$. Therefore at \tilde{q}_0 there is PT from a gapless spin-liquid into a gapless AF pseudo-spin-1/2 chain. At the phase transition the exponent γ jumps to -1 [29]. We have determined at $g = 0$ the critical value $\tilde{q} \simeq 1.35$, in good agreement with the expected value. Our results are consistent with $1 - \tau \sim \sqrt{\tilde{q}_0 - \tilde{q}}$ when approaching the PT for growing q . Hence at $g = 0$ and \tilde{q}_0 there is a C-IC PT [33] between the two gapless phases. Moreover, $g = 0$ and \tilde{q}_0 is a multicritical point for three phases: spin-liquid, pseudo-spin-1/2 iHAF, and the dimerized phase.

The region $g < 0$ smoothly connects with $g = 0$ since perturbations from $g = 0$ into $g < 0$ are (marginally) irrelevant in the renormalization group (RG) sense [15] and the symmetry dynamically enlarges to $SU(4)$. One could hence expect that the $g < 0$ region behaves similarly to

the $g = 0$ case for growing q . There is, however, an important distinction, since for $g \neq 0$ τ is not a good quantum number, never saturating for finite q . The situation resembles that of electrons in an external magnetic field in the presence of spin-non-conserving processes, which are irrelevant in the effective description but explicitly break the microscopic symmetries of the lattice model spoiling magnetization as a good quantum number [34]. A plausible scenario for $g \leq 0$ is that the QZE induces a C-IC PT, so that chirality-non-conserving processes remain irrelevant all the way, and do not modify the nature of the PT which takes place at $g = 0$. Numerical simulations must be performed to confirm this scenario. The PT cannot be identified by studying τ , and instead we study γ [35]. A jump in γ , if present, will confirm the C-IC nature of the PT. At small $g < 0$ we obtain that the PT retains the main features of that at $g = 0$, and that indeed γ abruptly jumps into -1 (Figs. 1 and 2(b)).

In summary, the QZE strongly modifies the MI phases of hard-core spin-3/2 fermions. Interestingly, contrary to bosons, a large $SU(2) \otimes SU(2)$ symmetry remains at any q , resulting at large q in a gapless pseudo-spin-1/2 iHAF. For $g > 0$ our results suggest a KT PT from a gapped dimerized spin-3/2 phase into the iHAF. On the contrary, for $g \leq 0$ there is a PT between a gapless spin-liquid into the iHAF, which (at least for low $|g|$) belongs to the C-IC universality class. The phase diagram (Fig. 1) has a non-trivial asymmetry characterized by a re-entrant dimerized phase. We have studied various observables, as chirality and spin correlations, which may reveal these phases in future experiments. Note that spin-changing collisions provide a unique opportunity to study experimentally a field-induced C-IC PT in four-component fermions, contrary to two-component ones where a magnetic field cannot induce a C-IC PT due to the conservation of magnetization. Note also that a richer physics is expected for higher spins, e.g. 5/2, where we expect for growing q a sequential transition from a spin-5/2 into a pseudo-spin-3/2 and finally a pseudo-spin-1/2.

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