Ultracold Fermions and the SU(N) Hubbard Model

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We investigate the fermionic SU(N) Hubbard model on the two-dimensional square lattice for weak to moderate interactions using renormalization group and mean-field methods. For the repulsive case $U > 0$ at half filling and small N the dominant tendency is towards breaking of the SU(N) symmetry. For $N > 6$ staggered flux order takes over as the dominant instability, in agreement with the large-N limit. Away from half filling for $N = 3$ two flavors remain half filled by cannibalizing the third flavor. For $U < 0$ and odd N a full Fermi surface coexists with a superconductor. These results may be relevant to future experiments with cold fermionic atoms in optical lattices.

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After the celebrated observation of Bose-Einstein condensation [1] ultracold atom systems have received growing attention in the field of condensed matter physics. Recently, also quantum degenerate Fermi gases have been realized [2–5], opening up the possibility to study phenomena such as BCS superfluidity in a new context. As a further important advance, optical lattices have been used to realize the transition between a bosonic superfluid and a Mott insulator [6]. It has thus been demonstrated that cold atom systems can become a very flexible and clean laboratory for many exciting phenomena from the purview of condensed matter or interacting many particle systems. In particular, cold fermions in optical lattices may help to understand the notorious complexities of strongly correlated solid state systems such as the cuprate high-temperature superconductors [7].

Besides the realization of phenomena that are known to exist in some form in condensed matter systems, it is also interesting to ask whether the degrees of freedom offered by cold atoms could give rise to states of matter that do not have obvious counterparts in the physics of interacting electrons. Typical electron systems, at least in the first approximation, possess SU(2) spin rotational symmetry which can be broken spontaneously, leading to magnetic phenomena. For alkali atoms, the nuclear spin I and electron spin S are combined in a hyperfine state. Its total angular momentum F can be different from 1/2, and for each F there are $2F + 1$ hyperfine states differing by their azimuthal quantum number m_F. For example, for the fermionic ^{40}K, the nuclear spin is $I = 4$ and the lowest hyperfine multiplet (at weak fields) has $F = 9/2$. In magnetic traps only a subset of these $2F + 1$ states (the *low-field seekers*) can be trapped [2], but this constraint can be avoided by using all-optical traps [8].

In fact, the coexistence of the three hyperfine states $|F = 9/2, m_F = -5/2, -7/2, -9/2\rangle$ of ^{40}K in an optical trap has already been realized, with tunable interactions due to Feshbach resonances between $m_F = (-5/2)/(-9/2)$ and $m_F = (-7/2)/(-9/2)$, respectively [9]. A situation with strong attractive interaction among all three components can be realized, e.g., for the spin polarized states with $m_s = 1/2$ in ^{6}Li where the triplet scattering length $a = -2160a_0$ is anomalously large [10].

Optical lattices are created by a standing light wave leading to a periodic potential for the atomic motion of the form $V(x) = V_0 \sum_i \cos^2(kx_i)$, where k is the wave vector of the laser, i labels the spatial coordinates, and the lattice depth V_0 is usually measured in units of the atomic recoil energy $E_R = \hbar^2 k^2/2m$. In the following we consider the two-dimensional (2D) case where $i = 1, 2$. It has been shown [11] that the *Hubbard model* with a local density-density interaction provides an excellent description of the low-energy physics. Here we are interested in a situation where fermionic atoms with N different spin states (“flavors”) m are loaded into the optical lattice. We thus consider a Hubbard Hamiltonian

$$H = -t \sum_{m,\langle ij\rangle} [c^\dagger_{i,m} c_{j,m} + c^\dagger_{j,m} c_{i,m}] + \frac{U}{2} \sum_i n_i^2. \qquad (1)$$

Here $n_i = \sum_m n_{i,m}$ is the total number density of atoms on site i which can be written in terms of creation and annihilation operators, $n_{i,m} = c^\dagger_{i,m} c_{i,m}$. The interaction [second term in Eq. (1)] is invariant under local U(N) rotations of the N flavors with different m. The hopping term of the atoms between nearest neighbors $\langle ij\rangle$ reduces the invariance of H to a global U(N) symmetry. Stripping off the overall U(1) phase factor, we arrive at the SU(N) Hubbard model. In the optical lattice the Hubbard parameters are $t = E_R(2/\sqrt{\pi})\xi^3 \exp(-2\xi^2)$ and $U = E_R a_s k \sqrt{8/\pi}\xi^3$, where $\xi = (V_0/E_R)^{1/4}$. a_s is the s-wave atomic scattering length.

The fermionic SU(N) Hubbard model on the 2D square lattice was studied in the large-N limit [12] in the early days of high-T_c superconductivity, mainly as a controllable limit connected to the then physically relevant case $N = 2$. Already then, Affleck *et al.* [13] discussed realizations of SU(4) using the nuclear spin of ^{21}Ne. A generalized SU(N) model could describe degenerate orbitals in crystals, but in general different overlaps between the orbitals pointing in distinct lattice directions will break the SU(N) invariance.

In the following we focus on the density region near half band filling with an average of $N/2$ fermions per site. In the conventional $N = 2$ Hubbard model at half filling the ground state exhibits spin-density wave (SDW) order, and when the filling is changed d-wave superconductivity is very likely [14]. The SDW state breaks the translational invariance and spin-up and spin-down electrons (for staggered moment along the z direction) occupy the two sublattices differently (see Fig. 1). For large N and small exchange interactions J, staggered flux order is expected to dominate over the SU(N)-breaking states [12].

First we analyze the one-loop renormalization group (RG) flow for the half filled band. We apply the perturbative temperature-flow RG of Ref. [15] with a Fermi surface (FS) discretization using 48 patches that has proved to give good results for $N = 2$. As the initial condition we fix the interaction at a high temperature T of the order of the bandwidth. Then the RG flow describes the change of the interactions as T is lowered and perturbative corrections due to one-loop particle-hole and particle-particle processes are taken into account. The interaction is described by a coupling function $V(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ [16], where the flavor indices m_1 and m_3 of the first incoming particle with wave vector $\vec{k}_1$ and the first outgoing particle with $\vec{k}_3$ are the same. Similarly $m_2 = m_4$. As for $N = 2$, the RG flow goes to strong coupling. This means, as we start the flow at high T with a local interaction $V(\vec{k}_1, \vec{k}_2, \vec{k}_3) = U$, some couplings start to grow when T is reduced and finally leave the perturbative range. At this temperature scale we stop the flow and analyze which coupling constants grow most strongly. In analogy with the spin-1/2 case we consider couplings in the charge channel $V_c(\vec{k}, \vec{k}', \vec{q}) = NV(\vec{k} + \vec{q}, \vec{k}', \vec{k}) - V(\vec{k}', \vec{k} + \vec{q}, \vec{k})$ and in the SU(N)-breaking channel, $V_s(\vec{k}, \vec{k}', \vec{q}) = -V(\vec{k}', \vec{k} + \vec{q}, \vec{k})$, which, if divergent, signal a singular response for a small external field coupling to one of the generators of SU(N). We define FS averages, $\bar{V}^{\ell}_{c/s}(\vec{q}) = \oint_{\rm FS} d\phi_k \oint_{\rm FS'} \times d\phi_{k'} g_\ell(\vec{k}) g_\ell(\vec{k}') V_{c/s}(\vec{k}, \vec{k}', \vec{q})$. Here $g_1(\vec{k}) = 1$ for the s wave and $g_2(\vec{k}) = (\cos k_x - \cos k_y)/\sqrt{2}$ for the d wave.

For $N = 2$ the s-wave spin couplings $\bar{V}^s_s(\vec{Q})$ with $\vec{Q} = (\pi, \pi)$ diverge most strongly, indicating an antiferromagnetic (AF) SDW state. This picture remains the same up to $N \leq 6$, signaling a dominant tendency towards breaking of the SU(N) symmetry with staggered two-sublattice real space dependence. For $N > 2$ (especially for odd N) this leads to the interesting question how the $N/2$ particles per site will arrange themselves on the bipartite square lattice (see Fig. 1). Below we describe what happens in a mean-field analysis.

For $N > 6$ the flow to strong coupling changes qualitatively. Now the leading divergence is in the charge couplings $V_c(\vec{k}, \vec{k}', \vec{Q})$ with a $d_{x^2-y^2}$-wave dependence on $\vec{k}$ and $\vec{k}'$. $\bar{V}^d_c$ diverges more strongly than $\bar{V}^s_s$ (see Fig. 2), albeit at lower temperature $T \approx 0.014t$ for $U = 4t$ and $N = 7$. This signals a tendency towards staggered flux (SF) order with long-range ordering of the expectation value $\Phi_{\rm SF} = \sum_{\vec{k},m} (\cos k_x - \cos k_y) \langle c^\dagger_{\vec{k},m} c_{\vec{k}+\vec{Q},m} \rangle$. This result agrees with the large-N limit for small exchange interactions J [12]. The SF state has surfaced several times for the SU(2) case in connection with the high-T_c cuprates and related models [12,17], also as d-density wave state (although the particle density is *not* modulated). Its quasiparticles have a wave-vector-dependent energy gap that vanishes at $\vec{k} = (\pm\pi/2, \pm\pi/2)$ [18]. Nonzero $\Phi_{\rm SF}$ breaks translational and time-reversal symmetry with alternating particle currents around the plaquettes (see Fig. 1). If the particles were charged, their motion would give rise to alternating magnetic moments pointing out of the plane, hence the name staggered flux state. Note that $\Phi_{\rm SF}$ is SU(N) invariant and no continuous symmetries are broken. Correspondingly the SF state can order at finite temperatures in 2D. For the same reason it may be possible that the SF state sets in for somewhat lower N than the critical $N = 6$ in our one-loop RG study that neglects collective fluctuations.

Away from half filling the flow of the dominant (π, π) instability gets cut off at some low-energy scale that increases with the distance to half filling. Below there is a tendency towards $d_{x^2-y^2}$-wave Cooper pairing. However, the energy scales for pairing instabilities become very small with increasing N. Below we discuss pairing for $N > 2$ in the attractive case $U < 0$.

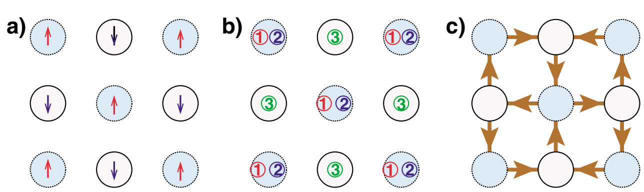

FIG. 1 (color online). (a) AF spin-density wave state for $N = 2$. Spin-up and spin-down particles occupy the two sublattices with different probabilities (here idealized to 0 and 1). (b) Flavor-density wave state for $N = 3$. Flavors 1 and 2 prefer one sublattice, flavor 3 the other. (c) Staggered flux state for $N > 6$: the arrows indicate the particle currents.

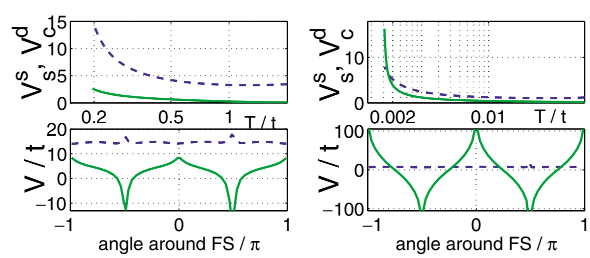

FIG. 2 (color online). Left plots: RG results for SU(3) at half filling and $U = 4t$. Upper left: flow of $\bar{V}^s_s$ in the SU(3)-breaking channel (dashed line) and $\bar{V}^d_c$ in the SF channel, averaged around the FS. Lower left: $V_s(\vec{k}, \vec{k}', \vec{Q})$ (dashed line) and $V_c(\vec{k}, \vec{k}', \vec{Q})$ with $\vec{k}$ fixed at $(\pi, 0)$ and $\vec{k}'$ moving around the FS. Right plots: the same for SU(8) at half filling.

Having established that SU(N) symmetry breaking at wave vector (π, π) is the dominant instability near half filling with $N < 6$, we now turn to a mean-field description of the ground state for $N = 3$. We decouple the interaction terms in the particle-hole channel with local mean fields $\langle c^\dagger_{\alpha,i} c_{\beta,i}\rangle = M_{\alpha\beta,i}$. The Hermitian local mean-field matrix $M_{\alpha\beta}$ can be decomposed into a traceful part M_0 proportional to the identity matrix t_0 and a traceless part $\sum_{a=1,\ldots,8} M^a t_a$ with the eight generators t_a of the fundamental representation of SU(3). A finite value of one of the traceless components breaks the SU(3) invariance. We now restrict the analysis to commensurate order, where only uniform and staggered components of a commuting subset of the nine M^a acquire nonzero expectation values. SU(3) has rank 2 and the two diagonal generators commute mutually and with the identity matrix. We can choose these 3 degrees of freedom to be contained in the three flavor-density mean fields $\langle n_\alpha\rangle$.

The results of $T = 0$ mean-field solutions are shown in Fig. 3. At half filling, $n = 1.5$ per site, the SU(3) breaking creates a flavor-density wave (FDW): two flavors prefer one sublattice with equal density, while the third flavor goes predominantly on the other sublattice with a somewhat larger density modulation. The staggered components do not add up to zero. Thus there is a charge-density wave accompanying the SU(3) symmetry breaking. For $U = 3t$ the mean field T_c for this state is $\sim 0.45t$, but in the one-loop RG it is reduced down to $\sim 0.12t$. Experimentally, the FDW and the resulting lattice period doubling can be detected by measuring the static structure factor $S(k)$ via flavor-dependent Bragg scattering [19] or in the particle density noise [20].

Figure 3 also describes the results away from half filling. For example, at $U = 1.6t$ and $1.42 < n < 1.48$ per site, two flavors order with opposite staggered densities on the two sublattices, keeping their individual average density at half filling. Since the total density is less than half filling, the third flavor gets decimated with uniform density of $(n - 1)$. As can be seen from the right plot in Fig. 3, this state occurs only above a critical interaction strength U_c that increases from zero with increasing distance to $n = 1.5$. The depletion of one flavor allows the system to preserve the commensurate order away from commensurate band filling. A similar pinning of a part of the system to half filling is found in ladder systems [21]. We add that for larger U and close to half filling ($1.46 < n < 1.5$ per site for $U = 4t$) we find another regime where the mean-field equations converge slowly and microscopic phase separation might occur.

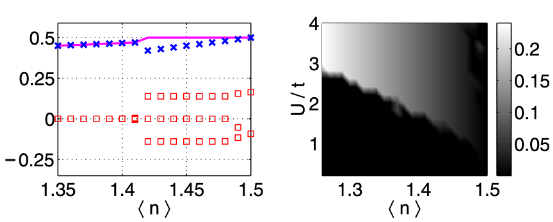

FIG. 3 (color online). Left: uniform densities of the $N = 3$ flavors (solid line: flavors 1 and 2; crosses: flavor 3) and staggered densities (squares) vs total density for $U = 1.6t$. Right: difference in uniform density between the two majority flavors and the minority flavor vs U and total density $\langle n\rangle$ per site. The scale bar indicates the density difference per site.

Next we consider attractive interactions $U < 0$. In the SU(2) case in 2D, there is a power-law s-wave singlet superconductor/superfluid (SSC) below a Kosterlitz-Thouless transition away from half filling [22]. At half filling T_c is zero, and SSC and charge-density wave (CDW) mean-field states are degenerate. In the true ground state, both orders coexist. One-loop RG finds in this case that CDW and SSC susceptibilities are degenerate and diverge together at low T. This symmetry is destroyed for $N > 2$, and the CDW susceptibility grows faster than the one for SSC. Correspondingly we expect the ground state to have CDW long-range order only. This is corroborated by a mean-field theory for SU(3) which shows that CDW order suppresses any SSC admixture, and that the CDW ground state has lower energy than the SSC state.

We now consider the generic case sufficiently far away from half filling. Then the dominant instability is on-site pairing. We decouple the interaction as $H_{U,\mathrm{mf.}} = \frac{1}{2}\sum_{\vec{k},\alpha,\beta} c^\dagger_{\vec{k}\alpha} c^\dagger_{-\vec{k}\beta}\Delta_{\alpha\beta} + \mathrm{H.c.}$ with the local mean fields $\Delta_{\alpha\beta} = -U\sum_{\vec{k}}\langle c_{\vec{k}\alpha} c_{-\vec{k}\beta}\rangle = -\Delta_{\beta\alpha}$. For $N > 2$ these even parity gap functions $\Delta_{\alpha\beta}$ transform nontrivially under SU(N). Depending on the global gauge, $\Delta_{\alpha\beta}$ takes different values. This is unlike the SU(2) case where even parity gap functions are singlets and invariant under spin rotations [23]. For SU(2) the ground state is degenerate with respect to the global phase of the gap function, and long-wavelength variations of the latter are gapless in the absence of long-range forces. In the SU(N) case we find a higher degeneracy and more gapless modes. It turns out that for SU(3) all gap functions with the same $\Delta_0^2 = \sum_{\alpha\beta}|\Delta_{\alpha\beta}|^2$ are degenerate and have the same total density of states. Apart from the global phase there are four additional gapless modes, two associated with the internal phases among Δ_{12}, Δ_{13}, and Δ_{23}, and two modes modulating $|\Delta_{12}|$, $|\Delta_{13}|$, and $|\Delta_{23}|$ with fixed Δ_0.

A particularly simple choice in the degenerate manifold is $\Delta_{12} = \Delta_0$ and $\Delta_{13} = \Delta_{23} = 0$. Then flavor 3 remains completely unpaired and metallic. Since we can always rotate into this gauge, all SU(3) s-wave superconducting mean-field states are one-third (neutral) metals and two-thirds superfluids. The gauge with only $\Delta_{12} \neq 0$ makes the symmetry breaking pattern obvious. The original symmetry group SU(3) ⊗ U(1) with nine generators gets broken down to an SU(2) in flavors 1 and 2, leaving Δ_{12} invariant, and an additional U(1) that acts on the phase of the unpaired flavor 3. This leaves five generators broken, yielding the collective modes described above. For 3/8 band filling and $U = 4t$, the mean field T_c is $\sim 0.17t$. The coexistence of a full FS with a superconductor should have interesting consequences. For example, the collective modes may be subject to damping below twice the gap frequency and could hence render the ungapped fermionic spectrum observable. Experimentally, these Goldstone modes can be detected in the spectrum of elementary excitations measured via Bragg scattering off two noncollinear laser beams with frequency and momentum difference ω, q [19]. By monitoring the number of scattered atoms, this technique yields the dynamical structure factor $S(q, \omega)$. The collective modes then lead to peaks in the scattering cross section.

Theoretically, an additional weak p-wave attraction could trigger a superfluid transition of the unpaired flavor at much lower temperatures, leading to a coexistence of even- and odd-parity superfluidity.

The SU(4) case is more complicated. There the degeneracy of the ground state is subject to more constraints than just constant Δ_0. The mean-field solutions have $|\Delta_{12}| = |\Delta_{34}|$, $|\Delta_{13}| = |\Delta_{24}|$. and $|\Delta_{14}| = |\Delta_{23}|$. The single particle spectrum is fully gapped.

In conlusion, the fermionic SU(N) Hubbard model on the 2D square lattice can possibly be realized with ultracold atoms in an optical lattice. Its ground states may exhibit phenomena that do not occur right away in traditional solid state systems. We find a staggered flux state for large $N > 6$ at half band filling where the particles run around the plaquettes of the lattice in an alternating way. This state has a partially gapped excitation spectrum with nodes along the Brillouin zone diagonals [18], which may be detectable via the momentum distribution function. Near half filling for $N = 3$ we find a redistribution of the particle densities where two of the three flavors remain half filled and occupy different sublattices while the third flavor becomes depleted. Finally, in the attractive case $U < 0$ we point out that the s-wave paired superfluid states may exhibit new collective modes. For $N = 3$ a third of the particles remains ungapped, leading to a full Fermi surface coexisting with the superfluid. We expect this to be a general feature for odd N, also in three dimensions or in the absence of a lattice potential.

Finally, we comment on the temperature scales which we have given in terms of the hopping parameter t. It has been shown [7] that if the optical lattice is switched on slowly after termination of evaporative cooling, an additional *adiabatic cooling* process takes place. The final temperature is given by the identity $T_{\mathrm{initial}}/T_{F,\mathrm{free}} \approx T_{\mathrm{final}}/T_{F,\mathrm{lattice}}$, where $T_{F,\mathrm{free(lattice)}}$ denote the Fermi temperature of the free atomic cloud and in the presence of the lattice, respectively. In particular, in 2D at half filling one has $T_{F,\mathrm{lattice}} = 4t$. As a result, the critical atomic temperatures which have to be reached *before* the lattice is switched on can be obtained from our results via the substitution $t \longrightarrow T_{F,\mathrm{free}}/4$. For the s-wave superfluid phase ($U < 0$) and the flavor-density wave states ($U > 0$) we therefore find transition temperatures of order $0.05T_F$ which are within reach experimentally.

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