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 interaction strengths using one-loop 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 \(N = 3\) the system rearranges the particle densities such that two flavors remain half filled by cannibalizing the third flavor. In the attractive case and odd \(N\) a full Fermi surface coexists with a superconductor in the ground state. These results may be relevant to future experiments with cold fermionic atoms in optical lattices.

Introduction: After the celebrated observation of Bose-Einstein condensation \(^1\) ultracold atom systems receive growing attention in the field of condensed matter physics. Recently, also quantum degenerate Fermi gases have been realized \(^2\) \(^3\) \(^4\) \(^5\), 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 atoms 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, it has been suggested \(^7\) that 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.

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, at least in the first approximation, possess SU(2) spin rotational symmetry which can be broken spontaneously, leading to magnetic phenomena such as ferro– and antiferromagnetism. 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 \(m_F\). E.g. for the fermionic 40K, 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 \(^8\), but this constraint can be avoided by using all–optical traps \(^8\).

In fact, coexistence of the three hyperfine states \(|F = 9/2, m_F = -5/2, -7/2, -9/2\rangle\) of 40K 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 \(^8\). A situation with strong attractive interaction between 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 \(a = -2160 a_0\) 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 \(V(x) = V_0 \sum_k \cos^2(kx_i)\) where \(k\) is the wavevector of the laser, \(i\) labels the spatial coordinates and the lattice depth \(V_0\) is usually measured in units of the atomic recoil energy \(E_R = h^2 k^2 / 2m\). In the following we will consider the 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

\[
H = -t \sum_{m, \langle ij \rangle} \left[ c_{i,m}^\dagger c_{j,m} + c_{j,m}^\dagger c_{i,m} \right] + \frac{U}{2} \sum_i n_i^2 . \tag{1}
\]

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 according to \(n_{i,m} = c_{i,m}^\dagger c_{i,m}\). 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 the complete Hamiltonian to a global \(U(N)\) symmetry. Stripping off the overall \(U(1)\) phase factor, we arrive at the SU(\(N\)) Hubbard model. Note that in the optical lattice the effective Hubbard parameters are given by \(t = E_R (2/\sqrt{\pi}) \xi^3 \exp(\sqrt{2} \xi^2)\) and \(U = E_R a_s k \sqrt{8/\pi \xi^3}\) where \(\xi = (V_0 / E_R)^{1/4}\) and \(a_s\) is the \(s–wave\) atomic scattering length.

The fermionic SU(\(N\)) Hubbard model for \(U > 0\) on the two-dimensional (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 \(N = 2\). A generalized SU(\(N\)) model could describe orbitally degenerate electronic states in crystals, but it is likely that in these systems different overlaps between the orbitals pointing in distinct lattice directions break the SU(\(N\)) invariance.

In the following we focus on the density region near half band filling with an average \(N/2\) 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 \[^{13}\]. 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 $\[^{12}\].

One-loop renormalization group for the half-filled band and general $N$ and $U > 0$: First let us analyze the one-loop renormalization group (RG) flow for the half filled band. We apply the perturbative temperature-flow RG method of Ref. \[^{14}\] that has proved to give good results for $N = 2$. As initial condition one fixes the interaction at a high temperature of the order of the bandwidth. Then the RG flow describes the change of the interactions as the temperature 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 $V(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ \[^{15}\], where the flavor indices $m_1$ and $m_3$ belonging to the first incoming particle with wavevector $\mathbf{k}_1$ and the first outgoing particle with $\mathbf{k}_3$ are the same. Similarly $m_2 = m_4$.

The second outgoing wavevector $\mathbf{k}_4$ is fixed by momentum conservation on the lattice. As in the $N = 2$ case the RG flow goes to strong coupling. This means, as we start the flow at high temperatures with a purely local interaction $V(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = U$, some coupling functions start to grow when the temperature is reduced and finally leave the perturbative range. At this temperature scale we stop the RG flow and analyze which class of coupling constants grows most strongly towards low $T$.

In close analogy with the spin-$1/2$ case we consider couplings in the charge channel $V_c(\mathbf{k}, \mathbf{k}', \mathbf{q}) = NV(\mathbf{k} + \mathbf{q}, \mathbf{k}') - V(\mathbf{k}', \mathbf{k} + \mathbf{q}, \mathbf{k})$ and in the $SU(N)$ symmetry breaking channel, $V_S(\mathbf{k}, \mathbf{k}', \mathbf{q}) = -V(\mathbf{k}', \mathbf{k} + \mathbf{q}, \mathbf{k})$, which, if divergent, signals a singular response for a small external field coupling to one of the $N^2 - 1$ generators of $SU(N)$. We define averages over the Fermi surface, $\bar{V}_{c/l}(\mathbf{Q}) = \int_{FS} d\phi_{\mathbf{Q}} d\phi_{\mathbf{k}'} g_l(k) g_l(k') V_{c/l}(\mathbf{k}, \mathbf{k}', \mathbf{q})$ with $g_l(k) = 1$ in the $s$-wave channel or $g_2(k) = (\cos k_x - \cos k_y)/\sqrt{2}$ in the $d$-wave channel. For $N = 2$ the couplings $V_c(\mathbf{Q})$ in the $s$-wave channel with $\mathbf{Q} = (\pi, \pi)$ diverge most strongly, indicating the formation of an antiferromagnetic (AF) SDW state. Note that for larger $N$ the charge couplings can become quite large as they scale with $N$.

Analyzing the RG flows to strong coupling, the picture is as follows: for $N \leq 6$ the $s$-wave coupling function $\bar{V}_s(\mathbf{Q})$ is the strongest divergent family of coupling constants, signalling 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 $V_c(\mathbf{k}, \mathbf{k}', \mathbf{Q})$ with a $d_{x^2-y^2}$-wave dependence on $\mathbf{k}$ and $\mathbf{k}'$. $\bar{V}_d$ diverges more strongly than $\bar{V}_s$ (see Fig. 2), albeit at lower temperature $T \approx 0.014T_c$ for $U = 4t$ and $N = 7$. This signals a tendency towards staggered flux (SF) order with long range ordering of the expectation value $\Phi_{SF} = \sum_{k,m} (\cos k_x - \cos k_y)(\epsilon_{k,m}^c \epsilon_{k+m}^s + \epsilon_{k+m}^c \epsilon_{k}^s)$. 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 \[^{12, 16}\] also as $d$-density wave state (although the particle density is not modulated). Its quasiparticles have a wavevector-dependent energy gap that vanishes at $\mathbf{k} = (\pm \pi/2, \pm \pi/2)$. Nonzero $\Phi_{SF}$ 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 $\Phi_{SF}$ is $SU(N)$-invariant and no continuous symmetries are broken. Correspondingly the SF state can order at finite temperatures in 2D. For the same rea-
son it may be possible that the staggered flux 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 $(\pi, \pi)$-instability gets cut off at some low energy scale that increases with the distance to half filling. Below that scale 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 superfluid pairing for $N > 2$ in the attractive case $U < 0$.

**Ground state near half filling for $N = 3$:** Having established that SU($N$) symmetry breaking at wave vector ($\pi, \pi$) is the dominant instability of the repulsive model 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 $\langle c^\dagger_{\alpha i}, c_{\beta i} \rangle = M_{\alpha \beta}$. The hermitian local mean-field matrix $M_{\alpha \beta}$ can be decomposed into a traceful part $M_0$ proportional to the identity matrix and a traceless part $\sum_{\alpha=1,...,8} M^{\alpha \dagger} M^\alpha$ with the 8 generators $M^\alpha$ of the fundamental representation of SU(3). A finite value of one of the traceless components breaks the SU(3) invariance. We will now restrict the analysis to commensurate order, where only uniform and staggered components of a commuting subset of the 9 $M^\alpha$ 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 three 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, $n = 1.5$ site, the SU($3$)-breaking creates a flavor-density wave: 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 $\sim 0.12t$.

Fig. 3 also describes the results away from half filling. For example at $U = 1.6t$ and $1.42 < n < 1.48$/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 only occurs above a critical interaction strength $U_c$ that increases from zero with increasing distance to $n = 1.5$/site. Note that 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 [17]. We add that for larger $U$ and close to half filling $(1.46 < n < 1.5$/site for $U = 4t$) we find another regime where the mean field equations converge slowly and microscopic phase separation might occur.

**Attractive SU($N$) Hubbard model:** Next let us consider the 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 [18]. At half filling the Kosterlitz-Thouless $T_c$ is zero, and SSC and charge-density wave (CDW) mean field states are degenerate and in the true ground state, both types of order coexist. One-loop RG finds in this case that CDW and SSC susceptibilities are perfectly degenerate and diverge together at low $T$. This symmetry is destroyed for larger $N > 2$ and the CDW susceptibility grows much 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 calculation for the SU($3$) case that shows that the CDW order suppresses any kind of SSC admixture, and the CDW ground state energy is lower than that of 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 $H_{U,mf} = -\frac{U}{2} \sum_{\vec{k},\alpha,\beta} c^\dagger_{\vec{k}\alpha} c_{\vec{k}\beta} \Delta_{\alpha\beta} + h.c.$ 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 non-trivially 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 [19]. 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 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 with the same $\Delta^2 = \sum_{\alpha,\beta} |\Delta_{\alpha\beta}|^2$ 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 between $\Delta_{12}$, $\Delta_{13}$ and $\Delta_{23}$, and two modes modulating $|\Delta_{12}|, |\Delta_{13}|$ and $|\Delta_{23}|$ with fixed $\Delta_0$.

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)
beams with frequency and momentum difference measured via Bragg scattering off two non–collinear laser beams with frequency and momentum difference $\omega, q \not\equiv 2 \pi / a$. By monitoring the number of scattered atoms as a function of $\omega$, this technique yields the dynamical structure factor $S(q, \omega)$. The collective modes will 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 $\Delta_0$. 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.

**Conclusions:** 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. For $U > 0$ 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, 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 absence of a lattice potential.

Finally, a comment on the temperature scales which we have given in terms of the hopping parameter $t$. It has been shown 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 $T_{\text{initial}}/T_{\text{free}} \approx T_{\text{final}}/T_{\text{F, lattice}}$ where $T_{\text{F, free(lattice)}}$ 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 $T_{\text{F, lattice}} = 4t$. 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 $t \rightarrow T_{\text{F, free}}/4$. 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 experimental reach.

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