Ultracold gases of ytterbium: ferromagnetism and Mott states in an SU(6) Fermi system

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\textbf{Abstract.} It is argued that an ultracold quantum degenerate gas of ytterbium \textsuperscript{173}Yb atoms having nuclear spin $I = 5/2$ exhibits an enlarged SU(6) symmetry. Within the Landau Fermi liquid theory, stability criteria against Fermi liquid (Pomeranchuk) instabilities in the spin channel are considered. Focusing on the SU($n > 2$) generalizations of ferromagnetism, it is shown within mean-field theory that the transition from the paramagnet to the itinerant ferromagnet is generically first order. On symmetry grounds, general SU($n$) itinerant ferromagnetic ground states and their topological excitations are also discussed. These SU($n > 2$) ferromagnets can become stable by increasing the scattering length using optical methods or in an optical lattice. However, in an optical lattice at current experimental temperatures, Mott states with different filling are expected to coexist in the same trap, as obtained from a calculation based on the SU(6) Hubbard model.
1. Introduction

Recently, the Kyoto group has managed to cool down to quantum degeneracy five ytterbium isotopes [1]. The ytterbium atom has a closed-shell electronic structure in the ground state ([Xe] 4f\(^{14}\) 5s\(^{2}\) 1S\(_{0}\)), and hence its spin stems entirely from the nuclear spin, \(I\). The case of the fermionic species \(^{173}\)Yb is particularly interesting, as it has nuclear spin \(I = F = 5/2\). Hence \(2F + 1 = n = 6\), and the atom can be in six different internal states. At ultracold temperatures, experiments show that the scattering length is independent of the atom internal state [2]. This can be understood from the absence of electronic spin in the atomic ground state, and the extremely weak dependence of the inter-atomic potential on the atomic nuclear spin. Thus, whereas for a spin-5/2 fermion the Lee–Yang–Huang pseudo-potential depends on three scattering lengths [3], \(a^F_{s} = 0, 2, 4\), the previous observation implies that \(a^0_{s} = a^2_{s} = a^4_{s} = a_{s}\). Mathematically, the interaction part of the Hamiltonian becomes:

\[
H_{\text{int}} = \frac{4\pi \hbar^2}{M} \sum_{i < j = 1}^{N} \left[ a^0_{s} \mathcal{P}_0(ij) + a^2_{s} \mathcal{P}_2(ij) + a^4_{s} \mathcal{P}_4(ij) \right] \delta(\mathbf{r}_i - \mathbf{r}_j) = \frac{4\pi \hbar^2 a_{s}}{M} \sum_{i < j = 1}^{N} \delta(\mathbf{r}_i - \mathbf{r}_j),
\]

where \(M\) is the atom mass and \(\mathcal{P}_F(ij)\) the projector onto the state of total spin \(F\) for the pair of particles \(i\) and \(j\). Therefore, the kinetic and interaction terms have the same symmetry, that is, the initial SU(2) spin-symmetry of the Hamiltonian describing an ultracold gas of \(^{173}\)Yb atoms is enlarged to an effective SU(6) symmetry. This is particularly interesting since enlarged symmetries usually lead to additional spectral degeneracies [4], which in turn can lead to exotic (correlated) ground states and topological excitations [5]–[8].

The occurrence of SU(6) in an ultracold gas can also lead to new and interesting connections with high-energy physics, where SU(6) has been used to describe the flavor symmetry of spinful quarks, as nuclear forces seem to be spin independent to a first approximation [4]. Indeed, some of the phases discussed below can be regarded as (non-relativistic) pion condensates that spontaneously break SU(6). In addition, these phases also bear some resemblance to the quantum Hall ferromagnets [8] discussed in two-dimensional electron gases with valley symmetry (such as graphene). Their possible existence in ultracold gases of \(^{173}\)Yb can allow for larger control, thanks to the large tunability of these atomic systems. In this regard, ultracold \(^{173}\)Yb atoms in optical lattices may also allow the observation of other exotic time-reversal symmetry breaking phases such as the staggered flux phase [9], which has been speculated as the explanation to the anomalous properties of the pseudo-gap phase of the high-\(T_c\) cuprate superconductors [10].
In this paper, we study (in section 2) the Fermi liquid instabilities in the spin SU(6) channel of a strongly interacting $^{173}$Yb gas. Focusing mainly on ferromagnetism, which breaks the SU(6) symmetry but not the space rotation invariance, we find in section 3 that the paramagnetic to ferromagnetic transition is generically first order for $n > 2$ at the mean-field level. On physical and symmetry grounds, we also identify the possible broken-symmetry ground states. The possibility of spontaneously breaking the SU(n) symmetry group in a cascade of phase transitions between different ferromagnetic phases hints at a much richer phase diagram than in the spin-$\frac{1}{2}$ case [12]. These phases will also sustain exotic topological excitations, such as skyrmions in two dimensions and monopoles in three dimensions. As argued below, these phenomena may be observed by increasing the scattering length using an optical Feshbach resonance [14] or perhaps also in a deep optical lattice. In section 4, we consider the situation in the lattice. Close to half-filling, i.e. three atoms per site, many phases, which may [6] or may not [9] break the SU(6) group, are likely to exist. However, at current accessible optical-lattice temperatures, atom hopping is largely incoherent, and Mott states are likely to coexist in the same harmonic trap. Indeed, as we show for an SU(6) Hubbard model at high temperatures, under the current experimental conditions the density profile will exhibit the Mott plateaux (see figure 3). Finally, a summary of the results as well as a brief discussion of how to detect some of the phases discussed here can be found in section 5.

2. SU(n) Fermi liquid and Fermi surface (FS) instabilities

We begin our analysis of the $^{173}$Yb system by exploring some consequences of SU(n = 6) for the Fermi liquid phase of an interacting gas of $^{173}$Yb atoms. Although we shall focus on the continuum case, many of the results in this section can be readily applied to the Fermi liquid phase of the gas loaded in an optical lattice (we neglect harmonic confinement for the moment; it will be considered briefly at the end, and more thoroughly elsewhere [16]). Following Landau [15], we describe the low-lying excited states of the system using the distribution function $n_\alpha^0(p) = \langle \psi_\alpha^0(p) \psi_\alpha^0(p) \rangle$ of a set of elementary excitations called Landau quasi-particles (QPs, essentially atoms ‘dressed’ by the interactions). Landau QPs are annihilated (created) by the Fermi operator $\psi_\alpha(p)$ ($\psi_\alpha^+(p)$) carrying (lattice) momentum $\hbar p$ and SU(n) index $\alpha = 1, \ldots, n$. The excitation free energy of the QP states is given by the Landau functional (summation over repeated Greek indices is implied henceforth): \[
\delta F = \sum_p \left[ \varepsilon_\alpha^0(p) - \mu \right] \delta n_\alpha^0(p) + \frac{1}{2\Omega} \sum_{p,p'} f^{\alpha\beta}_{\gamma\delta}(p,p') \delta n^\gamma_\alpha(p) \delta n^\delta_\beta(p'),
\] where $\Omega$ is the system volume and $\varepsilon_\alpha^0(p)$ is the excitation energy of a single Landau QP carrying momentum $\hbar p$. We assume the ground state to be an SU(n) singlet and therefore the ground state QP distribution $[n_\alpha^0]^0_\beta(p) = \theta(\mu - \varepsilon_\alpha^0(p))\delta^0_\beta$, where $\mu$ is the chemical potential; $\delta n^\alpha_\beta(p) = n^\alpha_\beta(p) - [n_\alpha^0]^0_\beta(p)$. The Landau functions $f^{\alpha\beta}_{\gamma\delta}(p,p') = f^{\beta\alpha}_{\delta\gamma}(p',p)$ describe interactions between QPs.

The above expression for $\delta F$ can be considerably simplified with the help of group theory by noting that $\delta n^\alpha_\beta(p)$ transforms as a tensor belonging to the reducible representation of SU(n) $n \otimes \bar{n} = 1 \oplus (n^2 - 1)$, where $n$ and $\bar{n}$ are the fundamental and complex conjugate representations, respectively, whereas 1 and $n^2 - 1$ are the singlet and the adjoint...

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components are determined by just two scalar functions (compared with the five needed for an $F = 5/2$ Fermi gas [3]), that is,

\[ f_{\gamma}^{\alpha \beta}(\mathbf{p}, \mathbf{p}') = f^{\alpha}(\mathbf{p}, \mathbf{p}') \delta_{\gamma}^{\alpha} \delta_{\beta}^{\beta} + 2 f^{m}(\mathbf{p}, \mathbf{p}') \sum_{a=1}^{n^2-1} (\mathbf{T})_{\gamma}^{a} (\mathbf{T})_{\delta}^{a}. \] (4)

We next consider the stability of the Fermi surface (FS) of the SU($n$) Fermi liquid just described above. For an isotropic FS, general stability conditions against FS deformations (Pomeranchuk instabilities (PIs), see figure 1) and pairing were obtained using the renormalization group by Chitov and Senechal [17]. They concluded that pairing occurs for attractive interactions. For repulsive interactions, $d$-wave pairing is also possible on a lattice near half-filling, but the pairing temperature rapidly decreases with increasing $n$ [6]. Therefore, the Fermi liquid phase should be a good starting description of the system. However, if the interaction is made sufficiently repulsive, the Fermi liquid can become unstable. The stability of the FS to the so-called PIs, that is, those instabilities for which the ground state of a Fermi system corresponds to a deformed FS (see figure 1), which is an FS that does not respect the space rotation symmetry (or lattice point group on a lattice) and/or spontaneously breaks internal symmetries such as the SU($n$) group discussed here, can be assessed within Fermi liquid theory. We shall next provide the SU($n$)-invariant extension of the Pomeranchuk stability criteria [15, 18] by considering the excitation energy of a QP distribution describing a deformation of the FS [15]. In matrix notation, $\pi(\mathbf{p}) = \theta(\mu - e^{0}(\mathbf{p})) \mathbb{1} + \delta u(\mathbf{\hat{p}})$, where $\pi(\mathbf{p})$ denotes the matrix whose components are $n^2(\mathbf{p})$, $\mathbb{1}$ is the unit matrix, and for this deformed distribution the matrix whose components are $\delta n^{a}_{\beta}(\mathbf{p})$ can be obtained from the following expression:\n
\[ \delta n^{a}_{\beta}(\mathbf{p}) = \frac{1}{n} \delta \rho(\mathbf{p}) \delta_{\beta}^{a} + \sum_{a=1}^{n^2-1} \delta m^{a}(\mathbf{p}) (\mathbf{T}^{a})^{a}_{\beta}, \] (3)

where $\mathbf{T}^{a}$ are the (traceless) generators of the SU($n$) Lie algebra obeying $[\mathbf{T}^{a}, \mathbf{T}^{b}] = i \sum_{c=1}^{n^2-1} \lambda^{abc} \mathbf{T}^{c}$; choosing the normalization such that $\text{Tr}(\mathbf{T}^{a} \mathbf{T}^{b}) = \frac{1}{2} \delta^{ab}$, the structure constants $\lambda^{abc}$ are fully anti-symmetric. In this representation, $\delta \rho(\mathbf{p})$ describes the total density fluctuations and $\delta m^{a}(\mathbf{p})$ the SU($n$) magnetization fluctuations. In the SU($n = 2$) case [15], equation (3) reduces to $\delta n^{a}_{\beta} = \frac{1}{2} \left[ \delta \rho(\mathbf{p}) \delta_{\beta}^{a} + \delta m(\mathbf{p}) \cdot \mathbf{\sigma}_{\beta}^{a} \right]$, where $\mathbf{\sigma} = (\sigma^{x}, \sigma^{y}, \sigma^{z})$ are the familiar Pauli matrices, and $\delta m$ is the usual magnetization vector. In addition, since the Landau functions transform as tensors belonging to $n \otimes n \otimes \hat{n} \otimes \hat{n} = 1 \oplus 1$ non-singlet representations, all the tensor components are determined by just two scalar functions (compared with the five needed for an $F = 5/2$ Fermi gas [3]), that is,

The step function $\theta(\mathbb{A})$, where $\mathbb{A}$ is a Hermitian matrix, should be mathematically defined as $\lim_{\beta \rightarrow 0} (e^{-\beta \mathbb{A}} - \mathbb{1})^{-1} = \theta(\mathbb{A})$. In particular, if $\mathbb{A}$ is diagonal, $\theta(\mathbb{A})$ is also a diagonal matrix whose elements are $\theta(\alpha_{\beta})$, where $\alpha_{\beta}$ are the eigenvalues of $\mathbb{A}$. Hence, $\theta(x \mathbb{1}) = \theta(x) \mathbb{1}$. Moreover, if $\mathbb{D} = U^{-1} \mathbb{A} U$, such that $\mathbb{D}$ is diagonal, then $\theta(\mathbb{A}) = U^{-1} \theta(\mathbb{D}) U$. Similar considerations apply to other distributions such as the Dirac delta function, etc.

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Figure 1. A Pomeranchuk instability (PI) occurs when the Fermi surface (FS) of an interacting Fermi system undergoes a permanent deformation from the state where the FS has all the symmetries of the Hamiltonian to a state where at least one of those symmetries is spontaneously broken. One example is a PI where the FS for all spin species becomes distorted in the same fashion (case a), thus breaking the space rotation symmetry. Another type (known as PI in the spin channel) corresponds to a situation where the FS corresponding to different spin species become distorted in a different fashion. A particular example of this type of PI is itinerant ferromagnetism (case b), which we study here for a Fermi gas possessing SU(6) symmetry.

whereas we only need to expand the SU(n) magnetization to the lowest order in \( \delta u \) because \( \delta F \) is already quadratic in \( \delta m^a \). Thus,

\[
\delta m^a(p) = \delta \left( \mu - \epsilon^0(p) \right) \delta u_m^a(\hat{p}) + \cdots.
\]  

Upon introducing these expressions into the Landau functional, equation (2), and working to second order in \( \delta u \), we arrive at the following expression after taking the thermodynamic limit (\( \Omega \to \infty \)):

\[
\frac{\delta F}{\Omega} = \frac{\delta F_\rho}{\Omega} + \frac{\delta F}{\Omega},
\]

\[
\frac{\delta F_\rho}{\Omega} = \frac{1}{2n} \int_{FS} d\hat{p} \left( \delta u_\rho(\hat{p}) \right)^2 + \frac{1}{2} \int_{FS} d\hat{p} d\hat{p}' \left( f^\rho(\hat{p}, \hat{p}') \right) \delta u_\rho(\hat{p}) \delta u_\rho(\hat{p}'),
\]

\[
\frac{\delta F_m}{\Omega} = \frac{1}{4} \int_{FS} d\hat{p} \sum_a \left( \delta u_m^a(\hat{p}) \right)^2 + \frac{1}{4} \int_{FS} d\hat{p} d\hat{p}' f^m(\hat{p}, \hat{p}') \sum_a \delta u_m^a(\hat{p}) \delta u_m^a(\hat{p}').
\]
where \( \int_{FS} dp \ldots = \int_{FS} dp \delta (\mu - e^0(p)) \ldots \) in an integral over the FS. In the continuum or in an optical lattice at low-filling, the FS is isotropic at the locus where \( |p| = p_F \), where \( p_F \) is the Fermi momentum. In three dimensions, we can expand
\[
\delta u_\rho(\mathbf{p}) = \sum_{LM} \delta u_{\rho,LM} Y_{LM}(\mathbf{p}) \quad \text{and} \quad \delta u_{\alpha,LM}(\mathbf{p}) = \sum_{LM} \delta u_{\alpha,LM} Y_{LM}(\mathbf{p}), f_{\rho/m}(p, p') = f_{\rho/m}(p \cdot \hat{p}) = \frac{\pi^{3/2}}{2L_m} \sum_{LM} f_{L_m}^{\rho/m} Y_{LM}(\mathbf{p}) Y_{LM}(\mathbf{p}),
\]
where \( Y_{LM}(\mathbf{p}) \) are the spherical harmonics. Therefore, \( \delta F = \delta F_\rho + \delta F_m \), where (note that \( \delta u_{\rho,LM}^\alpha, \delta u_{\alpha,LM}^\rho \) have units of energy)
\[
\frac{\delta F_\rho}{\Omega} = \frac{N^0(\mu)}{8\pi n} \sum_{LM} \left[ 1 + \frac{\mathcal{F}_L^\rho}{2L + 1} \right] |\delta u_{\rho,LM}^\alpha|^2,
\]
\[
\frac{\delta F_m}{\Omega} = \frac{N^0(\mu)}{16\pi} \sum_{LM} \left[ 1 + \frac{\mathcal{F}_m^\rho}{2L + 1} \right] \sum_a |\delta u_{\alpha,LM}^\rho|^2.
\]

We have introduced the (dimensionless) Landau parameters defined as \( \mathcal{F}_L^\rho = n N^0(\mu) f_L^\rho \) and \( \mathcal{F}_m^\rho = n N^0(\mu) f_m^\rho \), where \( N^0(\mu) = M^* p_F/(2\pi^2 \hbar^2) \) is the QP density of states (per species) at the FS in three dimensions, \( M^* = p_F (\partial \delta E/\partial p_F(p_F))^{-1} \) being the QP effective mass (\( M^* = M \), the bare atom mass in the Hartree–Fock approximation), and \( \hbar p_F \) the Fermi momentum, \( p_F = (6\pi^2 \rho_0 / n)^{1/3} \), where \( \rho_0 \) is the total density. Hence, from equations (10) and (11), the FS will be unstable if \( \mathcal{F}_m^{\rho/m} < -(2L + 1) \), for \( L = 0, 1, \ldots \).

The FS instabilities in the density channel (\( \delta F_\rho < 0 \), that is, \( \mathcal{F}_L^\rho < -(2L + 1) \)) are formally identical to those occurring in Fermi systems with no spin. They have received much attention recently [18], and lead to phases where the rotation (or point-group, in the lattice) symmetry of the FS is broken (\( L > 0 \)). On the other hand, much less attention has been focused on instabilities in the spin channel, which also break spin symmetry [19], and may occur in the interesting case of the \( ^{173}\text{Yb} \) system with SU\((n = 6) \) symmetry. Certainly, the most exotic states will be those resulting from an instability with \( L > 0 \) in the spin channel, or, for a non-isotropic FS, one that breaks the lattice point-group besides SU\((n) \). The resulting states have a much more complex order parameter, \( \Phi_{L,M}^\rho \propto \int d\mathbf{p} Y_{LM}(\mathbf{p}) (\mathbf{T}^a)_{\alpha/\beta} \delta n_{\beta}^a(p_F \mathbf{p}) \), that is the product of an orbital and an SU\((n) \) part (similar to superfluidity in \( ^3\text{He} \)).

However, as ultracold \( ^{173}\text{Yb} \) atoms naturally interact via repulsive s-wave (contact) interactions as the scattering length is \( a_s = +10.55 \text{ nm} \). This yields \( p_F a_s \approx 0.1 \) at the center of the trap in current experimental conditions [1, 20]. Furthermore, currently accessible temperatures \( T/\mu \approx 0.4 \) [1, 20] are well above any pairing temperature scale. In the isotropic case, \( \mathcal{F}_0^m \) is expected to be the most negative Landau parameter, thus favoring SU\((6) \) ferromagnetic correlations. Indeed, within Hartree–Fock theory, \( \mathcal{F}_0^m = N_0(\mu) g (n - 1) > 0 \), whereas \( \mathcal{F}_0^\rho = -N_0(\mu) g < 0 \) (\( N_0(\mu) = M p_F / (2\pi^2 \hbar^2) \)), where \( M \) is the atom mass, \( g = 4\pi \hbar^2 a_s/\mu M. \) Hence, the SU\((n) \) generalization of Stoner’s criterion for ferromagnetism, \( \mathcal{F}_0^m < -1 \), yields \( N_0(\mu) g > 1 \), or equivalently, \( p_F a_s > p_F a_s^* = \frac{\pi}{2} \), in the continuum case. It is worth noting that this criterion turns out to be the same for the SU\((2) \) case, that is, it is independent of \( n \). The independence of \( n \) of the Stoner criterion in an SU\((n) \) Fermi system can be understood using a simple energetic argument: to create a polarized ground state, imagine for example that \( \delta M_0/(n - 1) \) fermions are removed from the FS of each of the \( n - 1 \) flavors with \( \alpha < n \), and \( \delta M_0 \) are added to the FS of the \( \alpha = n \) flavor (so that the total particle number is unchanged). For small \( \delta M_0 \), the kinetic energy of the system increases by
\[
(n - 1) \frac{\delta M_0^2}{2\Omega N_0(\mu)} + \frac{(\delta M_0)^2}{2\Omega N_0(\mu)} = \frac{n(\delta M_0)^2}{2(n - 1)\Omega N_0(\mu)},
\]
whereas
the (Hartree–Fock) interaction energy decreases by $$\frac{n}{12} \left[ \frac{(n-1)(n-2)}{2} \left( \frac{\delta M_0}{n-1} \right)^2 - (n-1) \left( \frac{\delta M_0^2}{n-1} \right) \right] = -\frac{n\rho g^2}{2(n-1)^2 g^2}$$. Hence, upon comparing both energies, the dependence on $$n$$ drops out and the system becomes unstable provided that $$N_0(\mu)g > 1$$, which is independent of $$n$$ and agrees with the result obtained from the Fermi liquid theory within the Hartree–Fock approximation. The cancellation of the dependence on $$n$$ at the Hartree–Fock level is a consequence of the kinetic and exchange energies scaling linearly with $$n$$ (in spite of the fact that, naively, the interaction scales as $$n^2$$). Nevertheless, as we shall see below, the nature of the transition from a paramagnet to an itinerant ferromagnet turns out to be very different in an SU($$n > 2$$)-invariant Fermi system.

3. SU($$n$$) itinerant ferromagnets

The previous analysis using Landau Fermi liquid theory does not tell us anything about the order of the transition. In the spin-$$\frac{1}{2}$$ (SU(2)) case, the free-energy functional following from a microscopic calculation gives a continuous transition [11, 12]. However, it has been recently pointed out that the coupling of the order parameter fluctuations to soft modes changes the order of the transition from second to first order at low temperatures [12, 13]. In order to gain further insights into the nature of the transition at the mean field level, we shall derive in this section an effective action for the ferromagnetic order parameter starting from the microscopic model. To this end, we use the following operator identity for the interaction term of the Hamiltonian:

$$\mathcal{H}_{\text{int}}(\mathbf{r}) = \frac{1}{2}g \tilde{c}_\alpha(\mathbf{r}) c_\beta(\mathbf{r}) c^\beta(\mathbf{r}) c^\alpha(\mathbf{r}) = \frac{(n-1)}{2n} g [\rho(\mathbf{r})]^2 : -\frac{g}{2} \sum_{r=2}^{n} : \tilde{c}_\alpha(\mathbf{r}) (\mathbb{T}^{r-1})^a_\beta c^\beta(\mathbf{r}) :^2 :$$

(12)

In the above expression : . . . : stands for operator normal order, that is, the prescription that all atom creation fields, $$\tilde{c}_\alpha(\mathbf{r})$$, should stand to the left of the destruction fields, $$c^\alpha(\mathbf{r})$$. The matrices $$\mathbb{T}^{r-1} = \frac{1}{\sqrt{2n(r-1)}} \text{diag}(1, 1, \ldots, 1 - r, \ldots, 0, 0)$$ are the diagonal generators of the Lie algebra (i.e. the Cartan subalgebra). We next perform a Hubbard–Stratonovich decoupling of the density ($$\propto \rho^2$$) and SU($$n$$)-spin interaction terms, which yields the following action ($$\beta = 1/T$$, $$T$$ being the absolute temperature):

$$S[\tilde{c}_\alpha, c^\alpha, \varphi, \{\phi_r\}] = \int d\mathbf{r} \int_0^{\hbar \beta / h} d\tau \left\{ \frac{\hbar^2}{2M} \nabla^2 + \frac{n-1}{n} g \varphi(\mathbf{r}, \tau) \right\} \delta^\alpha_\beta - g \sum_{r=2}^{n} \mathcal{M}_r(\mathbf{r}, \tau) (\mathbb{T}^{r-1})^a_\beta c^\beta(\mathbf{r}, \tau) - \frac{n-1}{2n} g \varphi^2(\mathbf{r}, \tau) + g \sum_{r=2}^{n} \mathcal{M}_r^2(\mathbf{r}, \tau) \right\}. \quad (13)$$

Following the work by Hertz [11] for the SU(2) case, we focus on the SU($$n$$) spin fluctuations and therefore obtain an effective action for the fields $$\mathcal{M}_r(\mathbf{r}, \tau)$$ by integrating out the Fermions and setting the density-fluctuation field $$\varphi(\mathbf{r}, \tau) = \rho_0$$ ($$\rho_0$$ being the total density), that is, its saddle point value. Such a procedure yields the following effective action:

$$S_{\text{eff}}[\mathcal{M}] = -\text{Tr} \ln \left[ -G_0^{-1} - g \mathcal{M} \right] + g \int d\mathbf{r} d\tau \text{Tr} \mathcal{M}^2(\mathbf{r}, \tau), \quad (14)$$

where $$\mathcal{M}(\mathbf{r}, \tau) = \sum_{r=2}^{n} \mathcal{M}_r(\mathbf{r}, \tau) (\mathbb{T}^{r-1})$$, such that $$\text{Tr} \mathcal{M}(\mathbf{r}, \tau) = 0$$, and $$G_0^{-1}(\mathbf{r} - \mathbf{r}', \tau - \tau') = -(\hbar \partial_\tau - \mu + \frac{1}{n} g \rho_0 - \frac{\hbar^2}{2M} \nabla^2) \delta(\mathbf{r} - \mathbf{r}) \delta(\tau - \tau')$$. However, it should be noted that the present
Hubbard–Stratonovich decoupling scheme using only the diagonal generators of SU($n$) breaks the full SU($n$) invariance of the theory. Yet, it does reproduce the correct Stoner criterion in the mean field (Hartree–Fock) approximation, which, as discussed above, comes out to be independent of $n$. The SU($n$) invariance can be recovered by extending the functional integral over the entire set of traceless Hermitian matrices $\mathbb{M}$ transforming according to the adjoint representation of SU($n$). As noted in section 2, a convenient basis for this set is provided by the generators of the SU($n$) Lie algebra, $\mathbb{T}^a$, with $a = 1, \ldots, n^2 - 1$. Hence, $\mathbb{M}(r, \tau) = \sum_{a} m_a(r, \tau) \mathbb{T}^a$, where $m_a(r, \tau)$ are real fields. Near the paramagnetic–ferromagnetic phase transition, we expect the order parameter to be small and therefore, we perform a series expansion in $\mathbb{M}$ neglecting its dependence on $r$ and $\tau$. This yields the following (Landau) free-energy per unit volume:

$$
\frac{F}{\Omega} = \frac{F_0}{\Omega} + \sum_{j=2} \frac{g^j v_j}{j} \text{Tr} \mathbb{M}^j = \frac{F_0}{\Omega} + \frac{g^2}{2} v_2 \text{Tr} \mathbb{M}^2 + \frac{g^3}{3} v_3 \text{Tr} \mathbb{M}^3 + \frac{g^4}{4} v_4 \text{Tr} \mathbb{M}^4 + \cdots. \quad (15)
$$

The term of $O(g)$ vanishes identically because $\mathbb{M}$ is traceless. However, higher order terms proportional to $g^j$ with $j > 2$, for both even and odd $j$, occur in the free energy expansion in powers of $\mathbb{M}$ and cannot be ruled out. This is to be contrasted with the SU($n=2$) case, where only terms of even order occur [11]–[13] as consequence of time-reversal symmetry (and in the absence of a magnetic field). The coefficients $v_2 = (g^{-1} + \chi_2)$ and $v_j = \chi_j$ for $j > 2$, where $\chi_j = \langle -1 \rangle_{\beta} \sum_k \langle G_0(k) \rangle^j = -\frac{1}{(j-1)!} \frac{\partial^{j-2} N_0(\mu)}{\partial \mu^{j-1}}$, $k = (i\epsilon, \mathbf{k})$ and $G_0(k) = (i\epsilon - \epsilon(\mathbf{p}) + \mu)^{-1}$, where $\epsilon = \frac{2\pi}{\hbar} (l + \frac{1}{2})$, $\epsilon(\mathbf{p}) = \frac{\hbar^2 p^2}{2M}$, and we have shifted the chemical potential $\mu \to \mu - g\rho_0(n-1)/n$ to account for its renormalization due to interactions.

We could have obtained the above free energy based on symmetry considerations of the order parameter. However, the microscopic approach allows us to relate the coefficients of the expansion to the model parameters. We next set $\mathbb{M} = \sum_{a=1}^{n^2-1} m_a \mathbb{T}^a$ in (15) and use the following SU($n$) identity (see e.g. [22]):

$$
\mathbb{T}^a \mathbb{T}^b = \frac{1}{2n} \delta^{ab} \mathbb{1} + \frac{1}{2} \sum_{c=1}^{n^2-1} (d^{abc} + i f^{abc}) \mathbb{T}^c, \quad (16)
$$

where the group structure constants $d^{abc}$ are fully symmetric and $f^{abc}$ fully anti-symmetric [22]. For $n = 2$, $d^{abc} = 0$ but for $n > 2$ these structure constants are nonzero, which has important implications for the order of the paramagnetic–ferromagnetic phase transition. In terms of the $m_a$ components of the order parameter, the free energy reads as

$$
\frac{F}{\Omega} = \frac{F_0}{\Omega} + \frac{g^2}{4} v_2 \sum_a (m_a)^2 + \frac{g^3}{12} v_3 \sum_{abc} d^{abc} m_a m_b m_c + \frac{g^4}{16} v_4 \left\{ \frac{1}{n} \sum_a (m_a)^2 \right\}^2 + \frac{1}{2} \sum_{abde} d^{aeb} d^{cde} m_a m_b m_c m_d + \cdots. \quad (17)
$$

The above expression shows explicitly that the Landau free energy contains a cubic term in the order parameter $m_a$, which implies that, at least at the mean field level, the transition from the paramagnetic to the ferromagnetic phase is of the first-order type (see figure 2). Thus, the
system will exhibit hysteresis, and phase coexistence, with finite surface tension between the ferromagnetic and paramagnetic phases. Furthermore, the entropy will undergo a finite jump across the phase transition from the paramagnet to the SU(n) ferromagnet. The critical gas parameter resulting from Stoner’s criterion $p_F a_s^* = \frac{\pi}{2}$, which is the point where the quadratic coefficient vanishes, is actually larger than the actual critical value of the gas parameter, that is, $p_F a_s < p_F a_s^* = \frac{\pi}{2}$ (see figure 2). The latter corresponds to the point where both the paramagnetic minimum ($\mathbb{M} = 0$) and the ferromagnetic minimum ($\mathbb{M} \neq 0$) have the same free energy.

To illustrate the general ideas presented above, we shall next consider the case of the smaller group SU(3), which already contains essential ingredients of SU(n > 2) ferromagnetism. The more complicated case of SU(6) relevant to an unpolarized mixture of $^{173}$Yb atoms will be studied elsewhere [16]. However, it is worth saying that the SU(3) case would correspond to an experiment where the system is prepared as a mixture containing an equal population of only three of the six internal states.

Considering a three-dimensional gas in the continuum, setting $\mathbb{M} = U^\dagger (m_3 \mathbb{T}^3 + m_s \mathbb{T}^6) U$, where $U \in$ SU(3), and using cyclic property of the trace along with the parametrization $m_3 = \frac{(p_F a_s)^{-1}}{p_F} \tilde{m}_0 \cos \theta$ and

\begin{align*}
\text{Figure 2.} \quad \text{Generic mean-field phase diagram of an SU}(n > 2) \text{ interacting Fermi gas. For sufficiently repulsive interactions, the system undergoes a first-order phase transition from a paramagnetic state to a ferromagnetic state. The magnitude of the jump in the magnetization depends on the temperature and } n. \text{ Ferromagnetism is a Fermi surface (FS) instability that spontaneously breaks SU}(n) \text{ symmetry by making one of the FS for one species larger than the other } n-1 \text{ FSs.}
\end{align*}
\[ m_8 = \frac{(p_{\alpha})^{-1}}{\mu} m_0 \sin \theta, \]
we arrive at the following expression for the (dimensionless) free energy at \( T \ll \mu \):

\[
\frac{(F - F_0)/\epsilon_F}{p_{\beta}^2} = \frac{c_2}{2} \left( \frac{1}{p_{\alpha} a_s} - \frac{2}{\pi} \right) \tilde{m}_0^2 - \frac{c_3}{3} \tilde{m}_0^3 \sin 3\theta + \frac{c_4}{4} \tilde{m}_0^4 - \frac{c_5}{5} \tilde{m}_0^5 \sin 3\theta
\]

\[ + \frac{c_6}{6} \tilde{m}_0^6 (10 - \cos 6\theta) + \cdots. \]

In the above expression, \( \epsilon_F = \frac{\mu^2}{2M} \) is the Fermi energy, and the numerical coefficients are \( c_2 = 4\pi, c_3 = 8\pi/\sqrt{3}, c_4 = 16\pi^2/3, c_5 = 40\pi^3/3\sqrt{3} \) and \( c_6 = 16\pi^4/9 \). Using the above expression up to the sixth order, we can also obtain the shift in the critical gas parameter (relative to the Stoner value, \( p_{\alpha} a_s = \frac{\pi}{2} \)): \( (p_{\alpha} a_s')^{-1} - (p_{\alpha} a_s)^{-1} \approx 0.068 \) or \( 1 - a_s'/a_s \approx 0.097 \approx 10\% \) at the mean field level. Fluctuations are likely to decrease the critical value of the gas parameter even further from the Stoner value, and may also change the character of the transition (see e.g. [23]). In the SU(\( n > 2 \)) case, fluctuations are responsible for the change of the order of the transition for SU(2). Thus, further analysis of the effect of fluctuations is needed but it is beyond the scope of the present work.

For \( a_s < a_s' \), the free energy has one minimum located at \( \tilde{m}_0 = 0 \). However, for \( a_s > a_s' \) the free energy exhibits three degenerate minima, corresponding (in ‘Cartesian’ \((m_3, m_8)\) coordinates) to \( \tilde{m}_0 \propto (0, -1) \tilde{m}_0 \) and \( \tilde{m}_0 \propto (\pm \sqrt{3}/2, 1/2) \tilde{m}_0 \). However, it needs to be noted that these three minima represent the same physical state, as the result of the invariance of the free energy under the transformation \( \theta \to \theta + 2\pi j/3 \), where \( j = 1, 2 \), which corresponds to a cyclic permutation of the SU(3) indices \( 1 \to 2 \to 3 \to 1 \), or in other words, to the existence of three (non-commuting) SU(2) subalgebras in SU(3), into which the larger group SU(3) can be spontaneously broken. Thus, let us choose \( \tilde{m}_0 \propto -\tilde{m}_0 T^8 = -\tilde{m}_0 (1 - 3 e \otimes e) \) (corresponding to \( m_3 = 0 \) and \( m_8 = -m_0 \)), where \( e^i = (0, 0, 1) \). This ferromagnetic state corresponds to a gas where one of the species FS (\( \alpha = 3 \), in this case) grows at the expense of the two others, which remain degenerate. This state is left invariant under the transformations generated by the SU(2) subalgebra span by \( \{T^1, T^2, T^3\} \). Furthermore, it is left invariant by the U(1) transformations generated by \( T^8 \). Thus, the little group of transformations leaving the ground state invariant is SU(2) \( \otimes \) U(1). If the interaction is increased further on, the remaining SU(2) group may be also spontaneously broken down to U(1) in a subsequent transition.

Generally speaking, unlike the SU(2) case, the SU(\( n \)) may be spontaneously broken in a cascade of phase transitions. A general analysis of the possibilities can be given by considering the structure of the order parameter. As pointed out above, the order parameter is a traceless Hermitian matrix, \( \tilde{M} = \sum \tilde{m}_0 T^\alpha \), which transforms according to the adjoint representation of SU(\( n \)). Thus, when diagonalized, it has \( n - 1 \) independent eigenvalues. If only \( k < n \) of them turn out to be equal, the symmetry breaking pattern will be SU(\( n \)) \( \to \) SU(\( k \) \( \times \) [U(1)]\(^{n-k} \). Another more symmetric state occurs when there are only two distinct eigenvalues and hence SU(\( n \)) \( \to \) SU(\( n-k \)) \( \times \) U(\( k \)) (\( k \leq n/2 \)). When all the \( n-1 \) eigenvalues turn out to be different, SU(\( n \)) \( \to \) [U(1)]\(^{n-1} \), etc. A simple example of the broken symmetry ground states (at the Hartree–Fock level) is provided by the state \(|\Phi(p_1^k, \ldots, p_n^k)\rangle = \prod_{j=1}^{k} \prod_{|p|<\mu} c_j^a(p)|0\rangle \). Where \( |0\rangle \) is the particle vacuum. The number of different eigenvalues tell us how many of the Fermi momenta coincide. More generally, any ferromagnetic ground state can be considered to be adiabatically connected with an SU(\( n \)) rotation of \(|\Phi(p_1^k, \ldots, p_n^k)\rangle \). When there are only two
different eigenvalues, the order parameter manifold \( \mathcal{M} = G_{n,k} = SU(n) / [SU(n-k) \times U(k)] \), that is, a Grassmanian manifold \([8]\). In particular, for \( k = 1 \), \( G_{n,1} \simeq \mathbb{C} \mathbb{P}^{n-1} \), the complex projective space. These manifolds have nontrivial second homotopy group, \( \pi_2(G_{n,k}) = \mathbb{Z} (n \geq 2) \), which implies that these FM phases can sustain topologically stable excitations that are skyrmions in \( d = 2 \) and monopoles in \( d = 3 \). Furthermore, when \( SU(n) \) breaks into a subgroup containing more than one \( U(1) \), \( \pi_2(\mathcal{M}) = \mathbb{Z}^p \), where \( p \leq n - 1 \) is the total number of \( U(1) \)'s. The corresponding phases thus support complex types of topological defects described by several (integer) topological charges.

Finally, let us mention that as far as the experimental realization of \( SU(n > 2) \) ferromagnetism is concerned, the above discussion suggests that the most convenient approach to observe an \( SU(n > 2) \) paramagnet to ferromagnet phase transition in the \(^{173}\)Yb system is to increase the scattering length by means of an optical Feshbach resonance [14]. Ferromagnetism may also appear when the system is loaded in an optical lattice. However, this phase will compete with others (see next section) and further analysis will be required to understand the full phase diagram of the lattice system.

4. \(^{173}\)Yb gases in an optical lattice: \( SU(n = 6) \) Hubbard model

When the system is loaded in an optical lattice, other phases may become more energetically favorable. For a uniformly filled lattice, as the filling \( v = N/\mathcal{M} (N \text{ and } \mathcal{M} \text{ being the total atom and site numbers, respectively}) \) approaches half-filling, \( v = \frac{n}{2} \), many other phases are expected to occur [6, 9]. Let us assume that the optical lattice is sufficiently deep such that \(^{173}\)Yb gas on a lattice can be accurately described by a single-band Hubbard model:

\[
H = \sum_p \epsilon_0(p) c^\dagger_p(p) c_p(p) + \frac{U}{2} \sum_{\mathbf{R}} [\rho(\mathbf{R})]^2.
\]  

(18)

where \( \epsilon_0(p) = -2t \sum_{i=1}^{d} \cos k_i a_0 \) is the free particle dispersion (\( a_0 \) is the lattice parameter), and \( \rho(\mathbf{R}) = n^a_u(\mathbf{R}) \) the total site occupancy. One can also study anisotropic versions of this model by increasing the lattice depth along one direction so as to suppress hopping along this direction so that the system dimensionality becomes effectively \( d = 2 \). In this case, there is strong evidence that for large values of \( n \) [6, 9], a staggered flux phase [10] with atom currents circulating in opposite directions in neighboring plaquettes will be favored as the ground state. This phase breaks time-reversal as well as lattice translation symmetries but does not break \( SU(n) \). Thus, because the symmetry being broken is a discrete one, the system will exhibit long-range order also at finite temperatures in \( d = 2 \). In [6], it was argued that \( n = 6 \) is indeed a borderline case where this phase competes with a flavor density wave. The latter phase breaks both lattice translation symmetry and \( SU(n) \) symmetry. The order parameter for this phase is \( D^a_u(Q) = \frac{1}{2} \sum_p \langle c^\dagger_p(p) c^\dagger_{p+Q} \rangle \) (where \( Q = (\pi, \pi) \) at half-filling) and is also a tensor belonging to the adjoint representation. Thus, if \( \text{Tr} [D^a_u(Q) T^a] = D^a_u(Q) T^a \neq 0 \) for any \( a = 1, \ldots, n \), the \( SU(n) \) symmetry may be broken in one of the same patterns as in the FM case. Thus, the \(^{173}\)Yb gas in an optical lattice may be an ideal system to study the rich phase diagram resulting from the competition of all these phases. However, such a theoretical analysis of the full phase diagram is beyond the scope of the present work, and we refer the reader to the literature (see [6, 9] and references therein).

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However, the temperatures that are currently achievable in an optical lattice are well above the temperature scales where the ordered phases discussed above may occur. Indeed, as we argue below, assuming that the system is adiabatically loaded into the lattice, our calculations indicate that for the current experimental parameters, the temperature is larger (or of the same order, in the best case) of the hopping amplitude. Furthermore, the presence of harmonic confinement leads to an inhomogeneous filling of the lattice. The variation of the site occupation inside the trap, that is, the occupation profile, can be obtained for the current experimentally achievable temperatures, in the so-called atomic (i.e. \( t = 0 \)) limit of the SU\((n)\) Hubbard model introduced above upon accounting for the harmonic trap. In such a limit, the Hamiltonian reads:

\[
H_{at} = \frac{U}{2} \sum_{\mathbf{R}} \langle \rho (\mathbf{R}) \rangle^2 + V_t \sum_{\mathbf{R}} \left( \frac{\mathbf{R}}{a_0} \right)^2 \rho (\mathbf{R}),
\]

where \( V_t = \frac{1}{2} m \omega_0^2 a_0^2 \) is the trapping energy. The average site occupation can be thus obtained from the following expression:

\[
\langle \rho (\mathbf{R}) \rangle = \frac{\text{Tr} \left[ \rho (\mathbf{R}) e^{-(H_{at} - \mu N)/T} \right]}{\text{Tr} e^{-(H_{at} - \mu N)/T}},
\]

where \( N = \sum_{\mathbf{R}} \rho (\mathbf{R}) \) is the total particle number operator and \( T \) the absolute temperature. Hence,

\[
\langle \rho (\mathbf{R}) \rangle = T \frac{\partial}{\partial \mu} \ln \left[ \sum_{p=0}^{n} C_p^n \exp \left( -\frac{U}{2T} p^2 - \frac{V_t (\mathbf{R}/a_0)^2 - \mu}{T} p \right) \right],
\]

where \( C_p^n = \frac{n!}{p!(n-p)!} \) is the energy degeneracy of a single-site state containing \( p \) particles. The chemical potential \( \mu \) must be adjusted to fix the total number of particles and \( T \) must be such that the entropy of the lattice equals that of the gas before adiabatically ramping up the lattice. A plot of the site occupancy as a function of the radial distance to the center of the trap |\( R \)| is displayed in figure 3. In the lower panel of figure 3, we used parameters similar to those used in current experiments \[20\]. Thus, we find that the occupation at the center of the trap does not exceed two atoms per site and it would not be possible to directly observe the most important consequence of the SU\((n)\) symmetry on the lattice, namely the possibility that there are more than two (but at most six) atoms per site. However, the enhanced SU\((6)\) spin symmetry also increases, relative to the SU\((2)\) case \[24\], the entropy that is carried by the spin degrees of freedom of the \(^{173}\text{Yb}\) system. Thus, in order to observe larger occupation, the atom number and/or the trapping frequency and the entropy need to be changed. In particular, for the same atom number as used in the lower panel \((N = 10^4)\), we show that in the upper panel a slightly higher trapping frequency and a lower entropy per atom (i.e., lower temperature of the gas before being loaded into the lattice) would suffice to achieve half-filling near the center of the lattice. This could be a first step toward the observation of some of the exotic lattice phases discussed above, such as the staggered flux phase.

5. Summary and conclusions

To sum up, by using Fermi liquid theory, we have discussed Fermi liquid (Pomeranchuk) instabilities in the spin channel of a strongly interacting ultracold \(^{173}\text{Yb}\) gas exhibiting an...
Figure 3. Site occupation, $\rho(|\mathbf{R}|)$, as a function of the distance to the center of the cloud, $|\mathbf{R}|$, in units of the lattice parameter $a_0$, obtained from an SU(6) Hubbard model on a cubic lattice in $d = 3$. We have used parameters similar to those of current experiments [1, 20]. In both the upper and lower panels $U/t \simeq 45$ (lattice depth $10E_R$, $\omega_0$ is the trap frequency). The upper panel shows the emergence of a half-filled ($\rho(|\mathbf{R}|) = 3$) region near the center. The lower panel shows the emergence of the ‘Mott shell’ structure as the lattice entropy per atom is reduced. The red curve corresponds to the currently achievable temperatures of the gas (before adiabatically ramping up the lattice) of $T_{\text{init}}/T_F = 0.4$ [1, 20] ($T_F$ being the Fermi temperature of the harmonically trapped gas). The entropy is estimated using $(S/N)_{\text{latt}} = \pi^2(T_{\text{init}}/T_F)$, for a trapped non-interacting gas. For the smallest value of the entropy, $(S/N)_{\text{latt}} = 1.86$, the lattice temperature becomes comparable to the hopping (and therefore the atomic approximation breaks down). Hopping will further reduce the occupation near the edges of the cloud.
enlarged SU\( (n = 6) \) symmetry. Focusing on the ferromagnetic instability, which does not break space rotation or translation symmetries, we have shown that the transition is generically first order (at least, at the mean field level). Such an instability corresponds to a phase transition which can be observed by increasing the scattering length using an optical Feshbach resonance or/and in an optical lattice. For the continuum case, the first order of the transition implies that the transition takes places at a slightly smaller value of the scattering length than the value provided by the Stoner criterion, which we find to be independent of the order of the group, \( n \). Furthermore, using the smaller group SU(3) as an example, we have illustrated how the larger unitary symmetry is broken by an explicit analysis of the Landau free energy derived from the microscopic Hamiltonian. Thus, we found that SU(3) is spontaneously broken down to SU(2) \( \otimes \) U(1).

On general symmetry grounds, we can expect a number of symmetry-breaking patterns for SU(6), which may be the result of not just one but a cascade of phase transitions between ferromagnetic phases. These SU\( (n) \) ferromagnet systems can sustain exotic topologically stable excitations, such as skyrmions in \( d = 2 \) and monopoles in \( d = 3 \). The resulting phase diagram may be indeed quite rich, and will be explored elsewhere [16]. An interesting direction would also be to apply the analysis, based on Hertz theory [11], to study other FS instabilities in the SU\( (n) \) spin channel or to the flavor density wave [6] on the lattice. Based on the group theoretic properties of the order parameter, the latter may also turn out to be first order at the mean field level. Furthermore, in the optical lattice, the \(^{173}\)Yb system also offers other possibilities, such as a realization of the staggered flux phase, which breaks the lattice translation but not the SU\( (n) \) symmetry. However, under current experimental conditions, the temperature of the gas in the lattice is well above the ordering temperature for these phases. In this limit, we have obtained the density profile in a harmonic trap (see figure 3).

The fact that the spin of the ytterbium atom in its ground state is entirely nuclear implies that its coupling to a real magnetic field is very weak and this renders magnetic fields impractical for detecting the population of different species. However, the ferromagnetic phases and the topological defects discussed above could be detected by means of the optical Stern–Gerlach effect induced by off-resonant circularly polarized light [20]. Although this method has not yet been demonstrated experimentally, it provides the most direct way to image the population of each species in a single shot measurement [20]. Nevertheless, we hope that the possibilities discussed above for the observation of new and exotic many-body states in the \(^{173}\)Yb will spur further theoretical and experimental research along these lines. The first step in this direction may be measuring the site occupation in an optical lattice, which can be carried out as explained in [21].

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Note added. After completion of our work, we became aware of the work by Gorshkov et al [25], who also pointed out enlarged SU\( (n) \) symmetries of alkaline-earth atomic gases.

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