A single-band Hubbard model with nearest and next-nearest neighbour hopping is studied for $d = 1, 2, 3$, using both analytical and numerical techniques. In one dimension, saturated ferromagnetism is found above a critical value of $U$ for a band structure with two minima and for small and intermediate densities. This is an extension of a scenario recently proposed by Müller–Hartmann. For three dimensions and non-pathological band structures, it is proven that such a scenario does not work.

The Hubbard Hamiltonian, which has recently attracted so much interest as a model for describing high-$T_c$ superconductors, was investigated already in the sixties to face the problem of ferromagnetism in itinerant electron systems. Indeed, at a mean-field level, the Hubbard model seems to be a good starting point, as the Stoner criterion predicts a ferromagnetic ground state in a wide range of parameters. However, the inclusion of correlation effects makes the conditions for the appearance of ferromagnetism more stringent. The existence of large-spin ground states in Hubbard type models has been rigorously established in three different but rather peculiar situations: Nagaoka ferromagnetism for infinite $U$ and one hole in a half-filled band, Lieb ferromagnetism for half-filled bipartite lattices with sublattices containing a different number of sites, and the flat (or nearly-flat) band ferromagnetism of Mielke and Tasaki.

In a recent paper Müller–Hartmann proposed an alternative route to ferromagnetism. He considered the one-dimensional Hubbard model with both nearest- and next-nearest-neighbour hopping $(t_1-t_2$ Hubbard model). For infinite $U$ and a band dispersion with two degenerate minima he found saturated ferromagnetism for small electron densities. Very recently Penc and coworkers have studied a generalized version of Tasaki’s model in 1$d$ and found ferromagnetism in a large region of parameters. Their model reduces to that of Müller–Hartmann in a certain limit to which, however, their considerations do not apply.

In this paper we present numerical and variational results for the 1$d$ $t_1-t_2$ Hubbard model, which do confirm the existence of Müller–Hartmann ferromagnetism. Indeed we find that this phase is not confined to infinite $U$ and vanishingly small densities but occupies a substantial portion of parameter space. It is then natural to ask whether this route to ferromagnetism works also for higher dimensions. We will show that in dimensions $d > 2$ the answer is negative. For low enough densities (and a non-pathological band structure), even in the presence of several degenerate minima any state with finite magnetization is unstable. For the “marginal” dimension $d = 2$ we cannot exclude ferromagnetism but rather restrict strongly the region of its stability. In fact, the existence of many degenerate minima is not enough to stabilize the fully polarized state: what really matters is a high density of states at the bottom of the band.

We first consider the one-dimensional case. For the simple Hubbard model with only nearest-neighbour hopping, ferromagnetism has been discarded a long time ago by Lieb and Mattis, who showed that the ground state is a singlet. For the $t_1-t_2$ Hubbard chain

$$H = -\sum_{i,\sigma} (t_1 c_{i\sigma}^\dagger c_{i+1\sigma} + t_2 c_{i\sigma}^\dagger c_{i+2\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

the Lieb–Mattis theorem is not applicable since when $t_2 \neq 0$ the particles can pass each other and so cannot be ordered, which would be essential for the proof of the theorem. Actually, Mattis and Peña have shown that, when $t_1 > 0$ and $t_2 < 0$, the model shows Nagaoka ferromagnetism for one hole in a half-filled band. Here we are interested in small and intermediate densities.

We have performed numerical diagonalizations using the Lanczos method for chains up to $L = 18$ sites, for even electron numbers $N \leq L$ ($n = N/L$ is the electron density). The total spin of the ground state is determined both by measuring the spin–spin correlation function at $q = 0$ and by calculating the lowest energy states for each $S_z$ subspace. The energy of the fully polarized state is independent of $U$ and calculated analytically. When
t_2 > -t_1/4 (we always suppose t_1 > 0) the band has only one minimum at \( k = 0 \) and we do not find ferromagnetism at low density: for every value of \( U \) the ground state is a singlet. From now on we consider only the case \( t_2 < -t_1/4 \), when the band develops two degenerate minima at momenta \( \pm k_0 \), with \( k_0 = \arccos(t_1/4t_2) \). It is in this region that we should find, according to Müller–Hartmann, ferromagnetism at low density and infinite \( U \). We note that the lowest density that can be studied on a finite chain is \( 2/L \). For this case of two electrons, one can easily show that the ground state is a triplet. However, this result can be also regarded as an example of Mielke’s flat band ferromagnetism. Interestingly, for large enough \( U \), we do find ferromagnetism also for more than two electrons, namely for a range of densities up to a critical value \( n_c \). This is no longer flat band ferromagnetism but rather confirms the validity of Müller–Hartmann’s construction beyond the limit \( n \to 0 \) and \( U = \infty \).

In our numerical diagonalizations we have never found partially polarized ground states: the phase transition is always between a singlet and the fully polarized state. Fig.1 shows the behaviour of \( n_c \) as a function of \( t_2/t_1 \). Data from chains of different lengths are plotted in the following way: if for instance with \( N = 4 \) electrons the ground state is ferromagnetic, while with \( N = 6 \) it is not, we draw an error bar between \( 4/L \) and \( 6/L \). The solid curve represents the density at which the number of Fermi points for the fully polarized state changes from four to two. The curve seems to fit the data rather well and shortly, we are going to present an analytical argument that this is the likely criterion for the phase boundary. In any case, one can say that for densities above this curve Müller–Hartmann’s construction is no longer applicable since it relies on the existence of two disconnected pockets. In summary, our results indicate that this type of ferromagnetism is not restricted to very low densities, but it survives as long as the (fully polarized) Fermi sea has four Fermi points.

We turn now to the question which value of \( U \) is required to sustain ferromagnetism at a given density \( n \). Since our numerical results did not show evidence for a partially polarized ground state, we may examine the stability of the fully polarized state \( |F \rangle \) with respect to a single spin flip. We use the standard single-spin-flip trial state

\[
|\psi\rangle = \prod_i (1 - \eta n_{i\uparrow} n_{i\downarrow}) c_{k_0\downarrow}^\dagger c_{k_F\uparrow} |F\rangle.
\]  

(2)

An up-spin electron is removed from one of the Fermi points \( k_F \) (with energy \( \epsilon_F \)) and a down-spin electron is put to the bottom of one of the degenerate minima \( \epsilon_0 \) at wave vector \( k_0 \). This yields a single-particle energy gain of \( \Delta = \epsilon_F - \epsilon_0 \). The change of the total energy is

\[
\Delta E = -\Delta + Un \left( \frac{(1-\eta)^2}{1+(\eta^2-2\eta)n} + \frac{\eta^2}{1+(\eta^2-2\eta)n} \right)
\]

\[\cdot \left[ \epsilon_0(n^2-n) - \frac{E_0}{L} + \frac{E_1^2 \cos k_0}{2t_1L^2} + \frac{E_2^2 \cos 2k_0}{2t_2L^2} \right] \]  

(3)

where \( E_0 = E_1 + E_2 \) is the energy of the fully polarized state, while \( E_1 \) and \( E_2 \) are the contributions from the nearest-neighbour and next-nearest-neighbour hopping terms, respectively. \( \Delta E \) has to be minimized with respect to the variational parameter \( \eta \).

The polarized state becomes unstable when the kinetic energy gain outweighs the increased interaction energy. Fig.2. shows, for the special value \( t_2 = -t_1 \) the variational phase boundary \( U_{\text{var}}(n) \) (continuous curve) and the critical \( U_c \) determined by the numerical diagonalization (dots). We found similar results for other values of \( t_2 < -t_1/4 \). We notice that \( U_{\text{var}} \) is a lower bound for the exact \( U_c \). For small density \( n \), \( U_c \) decreases with decreasing \( n \), apparently tending to zero as \( n \to 0 \). The cusp of \( U_{\text{var}}(n) \) occurs at precisely the critical density we have defined above and indicates that something drastic happens there. While for \( n > n_c \), we see a sharply rising \( U_{\text{var}}(n) \), our numerical data indicate that ferromagnetism is completely suppressed in this region. Since the variational result provides a quickly increasing lower bound for \( U_c \), we take it as an indication that, in fact, \( U_c = \infty \) for \( n > n_c \). In this sense, the variational approach supports the phase diagram shown in Fig. 1.

We investigate now the stability of low-density ferromagnetism for \( d \geq 2 \). We consider the Hubbard Hamiltonian with arbitrary non-diagonal hopping terms \( t_{ij} \) and vanishing diagonal terms, \( t_{ii} = 0 \). However, we confine ourselves to non-pathological band structures, meaning quadratic dispersion about the minima. Since the most favourable situation for a fully polarized state is \( U = \infty \), we use the variational ansatz (2) for \( \eta = 1 \). A straightforward calculation gives

\[
\Delta E = -2n\epsilon_0 - \Delta + O(n^{1+2/d})
\]  

(4)

where \( \Delta = \epsilon_F - \epsilon_0 \sim n^{2/d} \). (In 1d, the leading correction would be \( O(n^2) \).) We note that \( \epsilon_0 \), the lowest eigenvalue of the hopping matrix, is necessarily negative, as the sum of the eigenvalues is equal to \( \sum_i t_{ii} = 0 \). The first term in Eq. (4) is therefore positive, favouring ferromagnetism, while the second term destabilizes the fully polarized state.

We examine now the viability of the low-density route for dimensions \( d > 1 \). For \( d \geq 3 \) the second term in (4) is the leading term at low density and the polarized state is always unstable for sufficiently low densities. (For \( d = 1 \) the first term is dominating and the present argument

\*At least for not too large \( |t_2| \). In fact, for \( |t_2|/t_1 \to \infty \), the system decouples into two simple Hubbard chains.
does not predict a destabilization of the fully polarized state.) For \( d = 2 \) the two terms are of the same order and must be compared more carefully. In this case, to leading order in \( n \), \( \Delta = n/\rho(\epsilon_0) \), where \( \rho(\epsilon_0) \) is the density of states at the bottom of the band. Inserting this expression into Eq. (4) and using the stability criterion \( \Delta E > 0 \), we obtain the following necessary condition for the stability of the fully polarized state,

\[
2\rho(\epsilon_0)|\epsilon_0| > 1. \tag{5}
\]

To be specific, let us consider the \( t_1-t_2 \) Hubbard model on a square lattice. When \( t_2 < -t_1/2 \) the band has degenerate minima at the Brillouin zone boundary. It follows from Eq. (5) that the polarized state cannot be the ground state outside the region \(-0.20t_1 > t_2 > -0.65t_1\). Hence for \( t_2 < -0.65t_1 \) the polarized state is unstable even though there are two minima.

Having excluded low-density saturated ferromagnetism for \( d > 2 \), we may wonder whether we can also say something about partially polarized states. Unfortunately, energy eigenstates with \( S < S_{\text{max}} \) are not exactly known, so that we have to find a different way for judging the stability of ferromagnetic order. An essential ingredient for the argument is the monotonous increase of the lowest energy eigenvalue as a function of \( U \), within any given subspace. This holds for the lowest singlet energy \( E_s(U) \) as well as for the lowest energy \( E_{pp}(U) \) within a subspace with a given partial polarization, as depicted in Fig. 3. An additional important fact is that the Hartree–Fock state gives an upper bound for the lowest energy eigenvalue as a function of \( U \).

We should comment on the relationship between our description of the low-density route to ferromagnetism and other scenarios of ferromagnetism in Hubbard models. The existence of the single-hole Nagaoka state is well-known, but it seems clear that the fully polarized state of the \( 1d \) \( t_1-t_2 \) model at low to intermediate densities is in its physical nature different, and in the phase diagram disconnected, from the Nagaoka state. In the special case \( n = 2/L \), our ferromagnetism is indistinguishable from Mielke’s but we find that the ordered state extends up to a \((t_2/t_1,\text{dependent})\) critical \( n_c \), and for finite concentrations \( n \) we certainly do not have flat-band ferromagnetism.

We have already mentioned that the generalization of Tasaki’s model \[8\] by Penc et al. \[10\] includes Müller–Hartmann’s model \[5\] as a special case. However, the understanding of ferromagnetism in \[10\] is based on the perturbative treatment of ring exchange processes, and this scheme breaks down for the model considered by us. Our finding that a decisive role is played by the existence of four Fermi points, seems to have no counterpart in their reasoning. The possible relationship between the ferromagnetic phase discussed in \[10\] and the one described by us, remains to be clarified.

It is worthwhile to point out that the existence of several degenerate minima does not play an essential role in our reasoning for \( d \geq 2 \). The phenomenon of valley-degeneracy-assisted ferromagnetism is apparently restricted to \( 1d \) systems.

To conclude, we have found an extended region of fully polarized ferromagnetic states in the \( U-n \) plane for the \( 1d \) \( t_1-t_2 \) model. The available evidence indicates that ferromagnetism exists whenever the Fermi sea consists of two disconnected parts. The ferromagnetism described by us is not a flat-band phenomenon, and it does not seem to be connected with the Nagaoka state, either. It is most unfortunate that the mechanism giving rise to the spin-polarized state in \( 1d \) does not work for non-pathological situations in \( 3d \) and has, at best, a rather restricted range of applicability in \( 2d \).

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\[8\] The \( t \)-matrix expansion has been also used to study the possibility of low-density ferromagnetism in the \( 3d \) and \( 2d \) Hubbard models \[4,5\]. Let us remark however that this expansion, even if physically justifiable, is nevertheless uncontrolled. Moreover, the role of several equivalent minima was not discussed. For the case of a single minimum, our results are in agreement with those of \[4,5\].
Figure Captions

Fig. 1. Phase diagram of the $t_1$–$t_2$ Hubbard chain in the $t_2$–$n$ plane, as obtained by exact diagonalization for finite lengths $L$. Circles: $L = 10$, diamonds: $L = 12$, squares: $L = 14$, triangles: $L = 16$. The full line shows the density where the fully polarized Fermi sea splits into two pockets.

Fig. 2. Phase diagram of the $t_1$–$t_2$ Hubbard chain in the $n$–$U$ plane, for $t_2 = -t_1$. Circles show numerical results, while the full line gives a variational lower bound. The location of the cusp ($n_c = 2/3$) corresponds to a point on the full line in Fig. 1.

Fig. 3. Schematic view of the $U$-dependence of the lowest energies for subspaces with different values of the total spin (s: singlet, pp: partially polarized). The dashed line shows the non-magnetic Hartree–Fock energy (HF).
Fig. 1
Fig. 2
Fig. 3