DMRG study of ferromagnetism in a one-dimensional Hubbard model

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Abstract

The one dimensional Hubbard model with nearest and (negative) next-nearest neighbour hopping has been studied with the density-matrix renormalization group (DMRG) method. A large region of ferromagnetism has been found for finite density and finite on-site interaction.

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1 Introduction

The Hubbard model was originally introduced to describe correlation effects in transition metals, such as, for example, the band ferromagnetism of Fe, Co and Ni. In mean field theory, one finds ferromagnetism whenever the Stoner criterion is satisfied, which, in the Hubbard model, leads to substantial regions of ferromagnetism in the phase diagram. When correlation effects are taken into account, however, a fully polarized ground state is quite difficult to find. For dimension $d = 1$, a theorem proven by Lieb and Mattis requires the ground state of the Hubbard model with near-neighbor hopping to be a singlet, completely excluding ferromagnetism [1]. For $d \geq 2$, ferromagnetism
is possible via the Nagaoka mechanism at very large interaction and near half-filling, but has not been found elsewhere in the phase diagram. Here we concentrate on the 1D case which can be extended to circumvent the Lieb–Mattis theorem so that ferromagnetism is allowed. One way to do this is to add orbital degeneracy to the model in order to mimic the Hund’s rule ferromagnetism found in atoms; another way is to add interaction terms such as nearest-neighbour Coulomb terms \([2]\). Finally, one can change the band structure by introducing a “flat band” \([3]\) or, as is done here, by adding longer range hopping terms.

## 2 Model and method

We will study the 1D Hubbard model with nearest and next-nearest-neighbour hopping:

\[
H = - \sum_{i=1,\sigma=\uparrow,\downarrow}^{L} (t_{1} c_{i\sigma}^{\dagger} c_{i+1\sigma} + t_{2} c_{i\sigma}^{\dagger} c_{i+2\sigma} + \text{h.c.}) + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}. \tag{1}
\]

Here \(c_{i\sigma}^{\dagger}\) creates an electron of spin \(\sigma\) on site \(i\), \(n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}\), \(L\) is the system size, and \(U\) is the on-site Coulomb interaction. In the following we express all energies in units of \(t_{1} = 1\) and only consider negative values of \(t_{2}\). Because a definite order of the particles is no longer enforced when \(t_{2} \neq 0\), the Lieb–Mattis theorem does not apply and, indeed, ferromagnetism has analytically been shown to exist at \(U = \infty\) in three different limits: For one hole in a half-filled band Nagaoka ferromagnetism has been found \([4]\); for \(|t_{2}| \to 0\), it has been shown \([5]\) that the model is ferromagnetic for all densities; and for \(|t_{2}| > 0.25\), where the band structure has two minima, Müller-Hartmann \([6]\) has shown that the low density limit is ferromagnetic. These three limits are indicated in the schematic phase diagram shown in Fig. 1. In addition, for \(|t_{2}| \to \infty\) the model can be mapped onto two decoupled Hubbard chains, which cannot be ferromagnetic due to the Lieb–Mattis theorem. The aim of this work is to determine the extent of these domains of ferromagnetism in \(n\) and \(U\), and whether or not these regimes are connected.

Previous work using Lanczos exact diagonalization and variational techniques with various trial functions \([7, 8]\) has shown that the ferromagnetic domain is large. However, the exact diagonalization calculations in this work
showed large finite size effects associated with closed shell effects in momentum space. Here we use the density matrix renormalization group (DMRG) method developed by White [9] and now widely used, to obtain results for much larger system sizes using open boundary conditions.

3 Results

Since the ground state energy obtained in the DMRG, $E_D$, is variational, it provides an upper bound for the exact ground state energy. We can analyse the stability of the fully polarized state by comparing its energy, $E_F$, which is exactly known since the state has no double occupancy, with $E_D$. For a given value of $t_2$ and density $n$ we can find a critical value $U_c$ below which the ferromagnetic state is unstable. Since $E_D$ can be found with high precision for this model, $U_c$ can be determined accurately. To check this we have calculated the total spin $S$ in the DMRG ground state by evaluating

$$\langle S^2 \rangle = \sum_{i,j} \langle S_i S_j \rangle.$$  \hspace{1cm} (2)

We find that the value of $S$ goes smoothly from 0 to the fully polarized value $S_{\text{max}}$ at the $U_c$ found by comparing the energies. It is difficult to determine whether the change in $S$ is continuous or not. The near–degeneracy of states with different $S$ at the transition leads to mixing of states in the diagonalization step of the procedure, so that $\langle S^2 \rangle$ no longer takes on definite discrete values. Using these two tools we have calculated the $U = \infty$ phase diagram shown in Fig. 2. The full dots are points at which the ground state is fully polarized (i.e. $E_D > E_F$ and $S \approx S_{\text{max}}$); the empty squares are points where the system is not magnetic (i.e. $E_D < E_F$ and $S \approx 0$); and the dashes are points at which the ferromagnetism is not fully saturated (i.e. $E_D > E_F$ and $S \neq S_{\text{max}}$). We can see that the previous analytical limits are well reproduced in this phase diagram and that the regions associated with the three mechanisms are connected.

We next examine the behavior at finite $U$. In Fig. 3, we choose three representative values of $t_2$ ($-0.1, -0.8, -2.0$), and show $U_c$ as a function of the density $n$. At $t_2 = -0.1$, the band has only one minimum, at $t_2 = -2.0$ the ferromagnetic region does not occur for all densities at $U = \infty$, and $t_2 = -0.8$ is intermediate between the two regions. We see that for the two cases in
which there are two minima ($|t_2| > 0.25$) in the band structure, there is a local minimum in $U_c$ at a given density $n_c$. This density corresponds to the Fermi level being just at the top of the barrier between the two band minima, which leads to a high density of states, favourable for ferromagnetism.

4 Conclusion

We have found a ferromagnetic ground state in a large parameter regime in the 1D Hubbard model with next-nearest neighbor hopping, showing that ferromagnetic regimes found in particular limits at $U = \infty$ extend to finite $U$ and density. We also find that these different ferromagnetic regimes are connected. One interesting unresolved issue is whether the transition from a paramagnetic to a ferromagnetic state is continuous. This issue can be clarified in future work by looking at appropriate correlation functions in more detail. The present results confirm that the “critical density” $n_c$ introduced in previous work [7] does not represent a true phase boundary [8], but merely a density where the $U$ value needed to stabilize ferromagnetism becomes small.

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References

[1] E. Lieb and D. C. Mattis, Phys. Rev. 125, 164 (1962).
[2] R. Strack and D. Vollhardt, J. Low Temp. Phys. 99, 385 (1995).
[3] A. Mielke and H. Tasaki, Commun. Math. Phys. 158, 341 (1993); H. Tasaki, Phys. Rev. Lett. 73, 1158 (1994);
[4] D. C. Mattis and R. E. Peña, Phys. Rev. B 10, 1006 (1974).
[5] M. W. Long, C. W. M. Castleton and C. A. Hayward, J. Phys. Condens. Matter 6, 481 (1994); K. Ueda, T. Nishino and H. Tsunetsugu, Phys. Rev. B 50, 612 (1994)

[6] E. Müller-Hartmann, J. Low. Temp. Phys. 99, 349 (1995).

[7] P. Pieri, S. Daul, D. Baeriswyl, M. Dzierzawa and P. Fazekas, Phys. Rev. B 45, 9250 (1996).

[8] S. Daul, P. Pieri, D. Baeriswyl, M. Dzierzawa and P. Fazekas, Physica B, in press.

[9] S.R. White, Phys. Rev. B 69, 2863 (1992); Phys. Rev. Lett. 48, 10345 (1993).

Figure captions

Fig. 1
Schematic $U = \infty$ ground state phase diagram in $n - t_2$ plane.

Fig. 2
The full dots show a ferromagnetic ground state, the open squares are for paramagnetic ground state, and the dashes are for points where doubts remain. The energy and $S$ where calculated on a system of size $L = 30$ at $U = 10^6$.

Fig. 3
Critical value of $U$ above which ferromagnetism is found for three different values of $t_2$, namely $t_2 = -0.2$ (full dots), $t_2 = -0.8$ (open squares) and $t_2 = -2$ (stars). The lattice size is $L = 50$. 
Fig. 1
Fig. 2
Fig. 3