

# Orbital order in a spin-polarized two-band Hubbard model

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## Abstract

In this work we prove the existence of a new phenomenon in the orbital order of a spin-polarized two-band Hubbard model, evaluated with the Gutzwiller approximation. This phenomenon is a transition in the orbital polarization which occurs continuously for arbitrarily weak interaction and involves a small fraction of electrons.

We obtain an explicit expression for the magnitude of the orbital polarization and analyze its dependence on the interaction constant  $U$  and the hopping constants  $t_\nu$  of the bands. Furthermore we show that the effect is not present in the Hartree-Fock approximation and that in particular cases it also disappears in the Gutzwiller approximation.

Finally we present numerical results for the semi-elliptic density of states and find agreement with the analytical results for weak interaction.



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# 1 Introduction

In this work we investigate a spin-polarized two-band Hubbard model. We assume that the spin-polarization is due to Hund's rule coupling. Takahashi and Shiba [1] used a simplified two-band Hubbard model to describe this two-band system where the spins in both bands are aligned. Motivated by the finding of a new continuous transition in the orbital order of such a system in one dimension achieved by Greger [2], we investigate if this effect is also present in a general Gutzwiller approximated system. The work is therefore also highly linked to the article [3], where, also by the use of the Gutzwiller variational method, orbital-order transitions in a three-dimensional system were investigated.

## 1.1 The Hamiltonian of a spin-polarized two-band Hubbard model

The Hubbard model was introduced 1963 by Hubbard [4], Kanamori [5] and Gutzwiller [6] as a highly simplified model which should capture important effects of the physics of transition-metal oxides. The general two-band Hubbard Hamiltonian looks like this:

$$\begin{aligned} \hat{H}_{\text{Hub}} = & \sum_{\mathbf{k}\nu\sigma} \epsilon_{\mathbf{k}\nu} \hat{a}_{\mathbf{k}\nu\sigma}^+ \hat{a}_{\mathbf{k}\nu\sigma} + U \sum_{i\nu} \hat{n}_{i\nu\uparrow} \hat{n}_{i\nu\downarrow} + V \sum_{i\sigma\sigma'} \hat{n}_{i1\sigma} \hat{n}_{i2\sigma'} \\ & + F \sum_{i\sigma\sigma'} \hat{c}_{i1\sigma}^+ \hat{c}_{i2\sigma'}^+ \hat{c}_{i1\sigma'} \hat{c}_{i2\sigma} + G \sum_{i\nu} \hat{c}_{i\nu\uparrow}^+ \hat{c}_{i\nu\downarrow}^+ \hat{c}_{i\nu\downarrow} \hat{c}_{i\nu\uparrow}, \end{aligned} \quad (1.1)$$

where  $\epsilon_{\mathbf{k}\nu}$  is the dispersion relation,  $\hat{n}_{i\nu\sigma}$  the density operator and  $\hat{a}_{\mathbf{k}\nu\sigma}^+$ ,  $\hat{a}_{\mathbf{k}\nu\sigma}$ ,  $\hat{c}_{i\nu\sigma}^+$ ,  $\hat{c}_{i\nu\sigma}$  are creation and annihilation operators in  $\mathbf{k}$ - and real space. The first term of the Hamiltonian describes the kinetic energy and the second ( $U$ ) the on-site interaction in each band. The third ( $V$ ), the fourth ( $F$ ) and the last ( $G$ ) term are due to the density interaction, the exchange interaction and pair hopping between two bands, respectively.

### The model in the ferromagnetic phase

We consider the situation that Hund's rule coupling aligns the spins in both bands. This can be achieved by choosing the responsible exchange constant  $F$  to be sufficiently large. The system then finds itself in a stable ferromagnetic phase in which for all electrons holds, say,  $\sigma = \uparrow$ . It now follows that we can neglect the energetically unfavorable  $\sigma = \downarrow$  states

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and consider only the  $\sigma = \uparrow$  sector of the Hamiltonian. The idea to consider this case with the in the following derived model Hamiltonian goes back to – as already mentioned above – Takahashi and Shiba [1].

In this situation the  $U$ - and the  $G$ -term yield zero as they describe hopping between states with different spin directions. We can then write (1.1) as an effective Hamiltonian reflecting the  $\sigma = \uparrow$  sector of  $\hat{H}_{\text{Hub}}$ :

$$\hat{H}_{\text{eff}} = \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}\nu} \hat{a}_{\mathbf{k}\nu\uparrow}^+ \hat{a}_{\mathbf{k}\nu\uparrow} + V \sum_i \hat{n}_{i1\uparrow} \hat{n}_{i2\uparrow} + F \sum_i \underbrace{\hat{c}_{i1\uparrow}^+ \hat{c}_{i2\uparrow}^+ \hat{c}_{i1\uparrow} \hat{c}_{i2\uparrow}}_{= -\hat{n}_{i1\uparrow} \hat{n}_{i2\uparrow}}. \quad (1.2)$$

We define  $\tilde{U}$  while assuming the following inequality to be fulfilled:

$$\tilde{U} := V - F > 0. \quad (1.3)$$

The assumption can be motivated by the fact that the relation  $U > V > F \cong G$  typically holds true.

Furthermore it is clear that the evaluation of (1.2) does not depend on the spin index  $\uparrow$ . We therefore define a new set of operators  $\hat{a}_{\mathbf{k}\nu}^+$ ,  $\hat{a}_{\mathbf{k}\nu}$ ,  $\hat{n}_{i1}$ ,  $\hat{n}_{i2}$  which corresponds to the operators used in (1.2) but lacks the spin index. This new set will now be used to analyze the spin-independent processes described by (1.2).

With the replacement of the operators in (1.2) by the according new operators and the definition of  $\tilde{U}$  we can finally write down the model Hamiltonian that is the starting point for this work:

$$\hat{H}_{\text{eff}} = \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}\nu} \hat{a}_{\mathbf{k}\nu}^+ \hat{a}_{\mathbf{k}\nu} + \tilde{U} \sum_i \hat{n}_{i1} \hat{n}_{i2}. \quad (1.4)$$

One sees immediately that this model Hamiltonian is formally equivalent to the one-band Hubbard model for fermions with different hopping constants for each spin direction (the only difference compared to our model is the replacement of  $\nu$  by  $\sigma$ ). In this analogy it is clear that we assume the dispersion relation for each band to have the same  $\mathbf{k}$ -dependence:  $\epsilon_{\mathbf{k}\nu} = t_\nu \tilde{\epsilon}_{\mathbf{k}}$ , but different hopping constants:  $t_1 \neq t_2$ . This situation – in contrast to the case  $t_1 = t_2$  – has still not been much investigated.

We will in the following drop the tilde of  $\tilde{U}$  in (1.4).

## 1.2 The variational method

Quantum-mechanical many-body problems can almost never be solved exactly. One approach to find solutions for them is to use variational wave functions. The general strategy



is to think about an explicit wave function

$$|\Psi_{\text{var}}\rangle = \hat{C}(\mathbf{g}) |\Phi_0\rangle, \quad (1.5)$$

where  $\hat{C}(\mathbf{g})$  is an operator which modifies the starting wave function  $|\Phi_0\rangle$  with respect to a set of variational parameters  $(g_1, \dots, g_n) \equiv \mathbf{g}$ . One usually wants to find the ground-state wave function, which is the one with the smallest energy eigenvalue of the system Hamiltonian. Therefore we try to get the optimized  $|\Psi_{\text{var}}\rangle$  by minimizing the expectation value of the Hamilton operator (known as the Ritz variational principle):

$$E_{\Psi_{\text{var}}} = \frac{\langle \Psi_{\text{var}} | \hat{H} | \Psi_{\text{var}} \rangle}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle}. \quad (1.6)$$

The obtained optimal wave function is of course not necessarily the true ground-state wave function, but is restricted to the chosen form of  $|\Psi_{\text{var}}\rangle$ . That is, the true ground state can perhaps not at all be arrived at, if one does not cover all possible  $|\Psi\rangle$  with the applied  $|\Psi_{\text{var}}\rangle$ . This naturally is hopeless in almost all cases.

Hence it is similarly unlikely to extract the true ground-state energy. Furthermore the corresponding  $|\Psi_{\text{var}}\rangle$  cannot be expected to reflect the physical nature of the problem in aspects other than the system energy.

Starting from the Hubbard Hamiltonian (1.4) we can immediately write down its energy expectation value per site (the division by  $L$  yields a simpler notation in following calculations):

$$E_{\Psi_{\text{var}}}^{\text{per site}} \equiv \frac{1}{L} \langle \hat{H}_{\text{Hub}} \rangle_{\Psi_{\text{var}}} = \frac{1}{L} \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}\nu} \langle \hat{a}_{\mathbf{k}\nu}^+ \hat{a}_{\mathbf{k}\nu} \rangle_{\Psi_{\text{var}}} + \frac{U}{L} \sum_i \langle \hat{n}_{i1} \hat{n}_{i2} \rangle_{\Psi_{\text{var}}}. \quad (1.7)$$

From now on we will always work with the energy per site and therefore drop the index:  $E_{\Psi_{\text{var}}} \equiv E_{\Psi_{\text{var}}}^{\text{per site}}$ . We make the common abbreviations for the occupancy  $n_{\mathbf{k}\nu}$  of a state  $|\mathbf{k}\nu\rangle$  and the double occupancy  $d$  of a site  $i$ :

$$n_{\mathbf{k}\nu}(\mathbf{g}) = \langle a_{\mathbf{k}\nu}^+ a_{\mathbf{k}\nu} \rangle_{\Psi_{\text{var}}} \quad (1.8)$$

$$d(\mathbf{g}) = \frac{1}{L} \sum_i \langle \hat{D}_i \rangle_{\Psi_{\text{var}}} \quad \text{where} \quad \hat{D}_i := \hat{n}_{i1} \hat{n}_{i2}. \quad (1.9)$$

These depend on  $\mathbf{g}$  because of their dependence on  $\Psi_{\text{var}}$ . Now the energy can be written as

$$E_{\Psi_{\text{var}}}(\mathbf{g}) = \frac{1}{L} \sum_{\nu\mathbf{k}} \epsilon_{\mathbf{k}\nu} n_{\mathbf{k}\nu}(\mathbf{g}) + U d(\mathbf{g}). \quad (1.10)$$

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### 1.2.1 The Hartree-Fock approximation

The fundamental approximation one makes in the Hartree-Fock approximation (HFA) is that the variational wave function  $|\Psi_{\text{var}}\rangle$  is taken to be an unchanged Slater determinant:

$$|\Psi_{\text{HF}}\rangle = \prod_{\mathbf{k}\nu, \epsilon_{\mathbf{k}\nu} \leq \epsilon_{\text{F}\nu}} a_{\mathbf{k}\nu}^+ |\text{vac}\rangle. \quad (1.11)$$

The Slater determinant form of the wave function makes up for two important characteristics of a quantum mechanical system. First, the indistinguishability of the particles and second, the Pauli principle.

We already stated that the resulting wave function still has the form of the uncorrelated starting wave function (the Fermi sea) as there actually is no explicit variational operator (what is optimized are the one-particle wave functions the Slater determinant is build up with). The occupancy of momentum space is therefore the same as in the non-interacting case, i.e.

$$n_{\mathbf{k}\nu} = \begin{cases} 1 & \text{for } \epsilon_{\mathbf{k}\nu} \leq \epsilon_{\text{F}\nu} \\ 0 & \text{for } \epsilon_{\mathbf{k}\nu} > \epsilon_{\text{F}\nu}. \end{cases} \quad (1.12)$$

Additionally the averaged product in (1.8) can – for the same reason – be split up:

$$\langle \hat{D}_i \rangle_{\text{HF}} = \langle \hat{n}_{i1} \hat{n}_{i2} \rangle_{\text{HF}} = \langle \hat{n}_{i1} \rangle_{\text{HF}} \langle \hat{n}_{i2} \rangle_{\text{HF}} \Rightarrow d = n_1 n_2.$$

Inserting these results in (1.10) gives the following expectation value for the energy:

$$E_{\text{HF}} = \frac{1}{L} \sum_{\nu, \epsilon_{\mathbf{k}\nu} \leq \epsilon_{\text{F}\nu}} \epsilon_{\mathbf{k}\nu} + U n_1 n_2. \quad (1.13)$$

where  $n_1, n_2$  are the expectation values for the electron density in the according band.

We state that the whole expression depends on  $U$  only in linear order and therefore refer to the HFA as an approximation linear in  $U$ .

### 1.2.2 The Gutzwiller wave function

For the Hubbard model, the simplest variational wave function of the form (1.5) was introduced by Gutzwiller 1963 [6]. The idea of it is to vary the double occupancy  $d$  in the starting wave function, which is inspired by the fact that interaction leads to a reduction of  $d$  compared to the uncorrelated case. One starts with the following ansatz for  $|\Psi_{\text{var}}\rangle$ :

$$|\Psi_{\text{G}}\rangle = g^{\sum_i \hat{D}_i} |\Phi_0\rangle = \prod_i \left[ 1 - (1-g)\hat{D}_i \right] |\Phi_0\rangle, \quad (1.14)$$

where  $g$  is a scalar variational parameter and  $|\Phi_0\rangle$  is the noninteracting Fermi sea, i.e. a Slater determinant. One immediately sees that  $g = 1$  yields the HFA and  $g < 1$  makes up for the reduction of  $d$ . It is equally clear that  $|\Psi_G\rangle$  covers up a tremendously bigger field of wave functions than the HFA, as it got rid of the fact that the starting wave function remains a Slater determinant throughout the whole variation process (this is accomplished by the operator  $\hat{D}_i$  which modifies the amplitudes of the one-particle wave functions in real space).

### 1.2.3 The Gutzwiller approximation

Besides introducing the wave function (1.14), Gutzwiller constructed an approximation scheme [6, 7] that allowed him to obtain an explicit expression for the ground state energy of the Hubbard model in terms of (1.14). This approximation (in the following called GA, see [8] for further explanation) was shown to be an exact evaluation of the Gutzwiller wave function in infinite dimensions by Metzner and Vollhardt [9, 10].

In this limit of infinite dimensions, the GA yields the following sectionwise constant occupancy of the momentum space [7]:

$$n_{\mathbf{k}\sigma} = \begin{cases} (1 - q_\sigma)n_\sigma + q_\sigma & \text{for } n_{\mathbf{k}\sigma}^0 = 1 \\ (1 - q_\sigma)n_\sigma & \text{for } n_{\mathbf{k}\sigma}^0 = 0 \end{cases} \quad (1.15)$$

where  $n_\sigma$  is the particle density for one spin and  $n_{\mathbf{k}\sigma}^0$  denotes the momentum distribution of the non-interacting Fermi sea. It is used to identify the position of the Fermi edge when interaction is turned off. The discontinuity  $q_\sigma$  at the Fermi edge is given by:

$$q_\sigma = \frac{\left(\sqrt{(n_\sigma - d)(d - n + 1)} + \sqrt{(n_\sigma - d)d}\right)^2}{n_\sigma(n_\sigma - d)}, \quad (1.16)$$

whereas the double occupancy  $d$  is related to the variational parameter  $g$  by:

$$g^2 = \frac{(1 - n + d)d}{(n_\uparrow - d)(n_\downarrow - d)}. \quad (1.17)$$

We recognize that  $d$  is an equally good variational parameter compared to  $g$ , but is easier to handle as it appears directly in the  $q_\sigma$  term. In the whole work we will therefore use  $d$  for further variational calculations. To apply these results to our model we simply change the index  $\sigma$  to  $\nu$ .

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We then insert (1.15) and (1.16) into (1.10) and end up with:

$$\begin{aligned}
 E_G(d) &= \frac{1}{L} \sum_{\nu} \left( \sum_{\mathbf{k}} n_{\mathbf{k}\sigma}^0 (\epsilon_{\mathbf{k}\nu} (1 - q_{\nu}(d)) n_{\nu} + q_{\nu}) + \sum_{\mathbf{k}} (1 - n_{\mathbf{k}\sigma}^0) \epsilon_{\mathbf{k}\nu} (1 - q_{\nu}(d)) n_{\nu} \right) + Ud \\
 &= \frac{1}{L} \sum_{\nu} \left( (1 - q_{\nu}(d)) n_{\nu} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}\nu} + q_{\nu}(d) \sum_{\mathbf{k}} n_{\mathbf{k}\sigma}^0 \epsilon_{\mathbf{k}\nu} \right) + Ud.
 \end{aligned} \tag{1.18}$$

Here the factors  $n_{\mathbf{k}\sigma}^0$  and  $(1 - n_{\mathbf{k}\sigma}^0)$  ensure the correct summation range (see (1.15)).

It is clear that the dependence of  $d$  on  $U$  – resulting from the variational process – can be rather complicated. Hence we expect that the GA is an approximation which is not linear in  $U$  as the HFA, but contains at least terms of order  $U^2$  for small  $U$ .

### 1.3 The density of states

For convenience in calculations we switch from the momentum space notation to a mathematical description in terms of the density of states (DOS)

$$\rho(\varepsilon) = \frac{1}{L} \sum_{\mathbf{k}} \delta(\varepsilon - \epsilon_{\mathbf{k}}). \tag{1.19}$$

We can use the following simple transformation for any sum over a function  $f(\epsilon_{\mathbf{k}})$ :

$$\begin{aligned}
 \frac{1}{L} \sum_{\mathbf{k}} f(\epsilon_{\mathbf{k}}) &= \frac{1}{L} \sum_{\mathbf{k}} f(\epsilon_{\mathbf{k}}) \underbrace{\int_{-\infty}^{\infty} d\varepsilon \delta(\varepsilon - \epsilon_{\mathbf{k}})}_{= 1} \\
 &= \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \underbrace{\frac{1}{L} \sum_{\mathbf{k}} \delta(\varepsilon - \epsilon_{\mathbf{k}})}_{= \rho(\varepsilon)} = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \rho(\varepsilon).
 \end{aligned} \tag{1.20}$$

We will need the particle density of one band:  $n_{\nu} = \frac{1}{L} \sum_{\epsilon_{\mathbf{k}\nu} \leq \epsilon_{F\nu}} 1$ . This becomes in the DOS description:

$$n_{\nu} = \int_{-\infty}^{\epsilon_{F\nu}} d\varepsilon \rho_{\nu}(\varepsilon). \tag{1.21}$$

In analogy to that, the average kinetic energy for each non-interacting band,  $\bar{\varepsilon}_{\nu} = \frac{1}{L} \sum_{\epsilon_{\mathbf{k}\nu} \leq \epsilon_{F\nu}} \epsilon_{\mathbf{k}\nu}$ , can be written as:

$$\bar{\varepsilon}_{\nu} = \int_{-\infty}^{\epsilon_{F\nu}} d\varepsilon \rho_{\nu}(\varepsilon) \varepsilon. \tag{1.22}$$

## 2 Definition of the model system

The aim of this work is to investigate the orbital order of the spin-polarized two-band Hubbard model for which the Hamiltonian was already given in the introduction. That means in our case that we try to find out if this system has a tendency to favor the residence of electrons in one of the bands. It was already stated that our model Hamiltonian is formally equivalent to that of a fermionic one-band Hubbard model. In this analogy the presence of orbital order in our system corresponds to a (ferromagnetic) magnetization  $m$  in the one-band Hubbard model. As the latter effect is the more familiar and more investigated one which already provides some useful results, it facilitates the discussion of orbital order if we treat it like a magnetization. In the following we will therefore do so and use the expression orbital polarization  $m$ .

Now it makes sense to write the energy no longer in terms of the occupancy of the bands, i.e. their particle densities  $n_1$ ,  $n_2$ , but in terms of the overall particle density  $n$  and the orbital polarization  $m$  by applying the substitution:

$$n = n_1 + n_2 \quad \text{and} \quad m = n_1 - n_2. \quad (2.1)$$

The problem that we encounter is the fact, that a two-band system with  $\epsilon_{\mathbf{k}1} \neq \epsilon_{\mathbf{k}2}$  is in general stable in a polarized state also if there is no interaction. We want to investigate the net influence of interaction on the orbital order. This effect is expected to be small compared to the magnitude of the initial orbital polarization of such a two-band system. For convenience in calculations and a higher numerical accuracy we therefore adjust our model system such that we obtain a nonpolarized ground state for  $U = 0$ . It is clear that this procedure makes our system quite synthetic. We will come back to that in the conclusion and restrict ourselves during this work to the model system defined below.

We require  $m = 0 \Leftrightarrow n_1 = n_2$  for the noninteracting state. In momentum space one can achieve that easily. We have already mentioned that the bands in our Hubbard model are supposed to have different hopping constants  $t_1$  and  $t_2$  for the possibilities of hopping from band 1 to band 2 and reverse ( $t_\nu$  will also be referred to as the kinetic energy scale of band  $\nu$ ). Besides that, the  $\mathbf{k}$ -dependence of the dispersion relation - which mirrors dimensionality and geometry of the lattice - is identical for each band. We therefore have:

$$\epsilon_{\mathbf{k}\nu} = t_\nu \tilde{\epsilon}_{\mathbf{k}} + C_\nu \quad (2.2)$$

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where we demand

$$\sum_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} = 0 \quad (2.3)$$

for convenience. The constant  $C_\nu$  was added to fulfill the requirement  $m \stackrel{U=0}{=} 0$  and will be determined now. As there is only one constraint to satisfy we can set  $C_1 = 0$ . As  $n_\nu = \frac{1}{L} \sum_{\epsilon_{\mathbf{k}\nu} \leq \epsilon_{F\nu}} 1$  depends on  $\nu$  only through  $\mathbf{k}_{F\nu}$  it follows (the superscript  $0$  will in the following course of the work indicate  $m = 0$ ):

$$n_1 = n_2 \Rightarrow \mathbf{k}_{F1}^0 = \mathbf{k}_{F2}^0 =: \mathbf{k}_F^0. \quad (2.4)$$

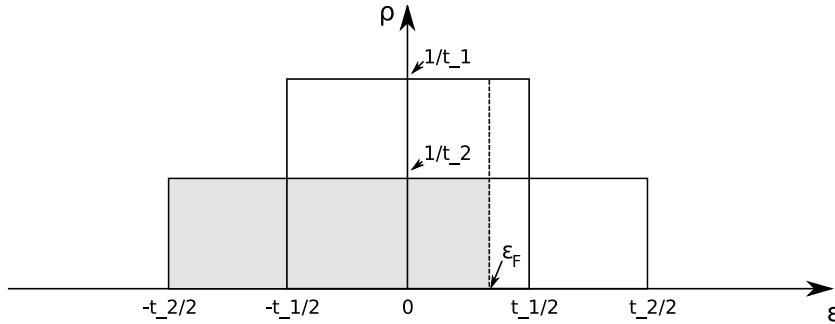
The Fermi energy then has to be identical for both bands:

$$\epsilon_{\mathbf{k}_{F1}^0}^0 = \epsilon_{\mathbf{k}_{F2}^0}^0 =: \epsilon_F^0. \quad (2.5)$$

Applying this, we can immediately determine  $C_2$  and summarize the results:

$$\begin{aligned} C_1 = 0 & \stackrel{(2.2)}{\Rightarrow} C_2 = (t_1 - t_2) \tilde{\epsilon}_{\mathbf{k}_F}^0 \\ & \stackrel{(2.2)}{\Rightarrow} \epsilon_F^0 = t_1 \tilde{\epsilon}_{\mathbf{k}_F}^0, \quad \tilde{\epsilon}_F^0 := \frac{\epsilon_F^0}{t_1} \equiv \tilde{\epsilon}_{\mathbf{k}_F}^0. \end{aligned} \quad (2.6)$$

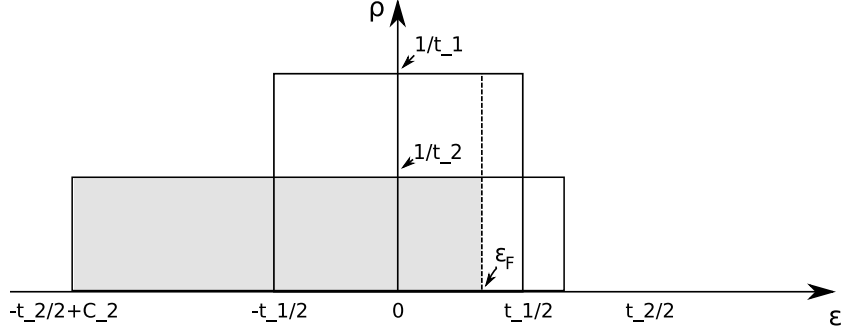
To use this result for the description of the system in terms of the DOS, we first look at an example. Fig. 2.1 shows an unadjusted system (corresponding to  $\epsilon_{\mathbf{k}\nu} = t_\nu \tilde{\epsilon}_{\mathbf{k}}$ ) with the constant DOS  $\rho_\nu(\epsilon) = \frac{1}{t_\nu}$ . The grey area is equivalent to the electron density in the second band  $n_2$ ; similarly  $n_1$  can be identified. It is obvious that  $n_2 < n_1$  holds and therefore the pictured system is polarized.



**Figure 2.1:** Two-band system with constant DOS

Now one sees from the definition of  $\rho$  that the explicit lower integration limit of the unchanged system is  $\epsilon_{\min\nu} = \min_{\mathbf{k} \in \text{BZ}} t_\nu \tilde{\epsilon}_{\mathbf{k}}$ , i.e. is the minimum of the image of the subset  $\mathbf{k} \in \text{BZ}$  under the function  $t_\nu \tilde{\epsilon}_{\mathbf{k}}$  (in Fig. 2.1:  $\epsilon_{\min\nu} = \frac{t_\nu}{2}$ ). It is then clear that a constant  $C_\nu$  added to the function  $t_\nu \tilde{\epsilon}_{\mathbf{k}}$  just corresponds to the same shift added to  $\epsilon_{\min\nu}$ . This

situation is pictured in Fig. 2.2.



**Figure 2.2:** Adjusted two-band system with constant DOS

We define the band-independent lower integration limit  $\tilde{\varepsilon}_{\min}$ :

$$\tilde{\varepsilon}_{\min} := \frac{1}{t_\nu} \varepsilon_{\min\nu}. \quad (2.7)$$

We will now calculate some expressions that will later be of use. Therefore we first exploit some well known properties of the delta function:

$$\begin{aligned} \rho_\nu(\varepsilon) &\stackrel{(1.19)}{=} \frac{1}{L} \sum_{\mathbf{k}} \delta(\varepsilon - \epsilon_{\mathbf{k}\nu}) \\ &\stackrel{(2.2)}{=} \frac{1}{L} \sum_{\mathbf{k}} \delta(\varepsilon - t_\nu \tilde{\varepsilon}_{\mathbf{k}} - C_\nu) \\ &= \frac{1}{|t_\nu|} \frac{1}{L} \sum_{\mathbf{k}} \delta\left(\frac{\varepsilon - C_\nu}{t_\nu} - \tilde{\varepsilon}_{\mathbf{k}}\right) \\ &\stackrel{(1.19)}{=} \frac{1}{|t_\nu|} \tilde{\rho}\left(\frac{\varepsilon - C_\nu}{t_\nu}\right) \end{aligned} \quad (2.8)$$

In the last step we achieved, in analogy to  $\tilde{\varepsilon}_{\mathbf{k}}$ , the band-independent expression  $\tilde{\rho}$  for the DOS. We will in the following consider only positive  $t_\nu$  which makes things easier and is no restriction to generality as the important quantity is the difference  $(t_1 - t_2)$ . We can now write  $n_\nu$  in the following way:

$$\begin{aligned} n_\nu &\stackrel{(1.21)}{=} \int_{\varepsilon_{\min\nu} + C_\nu}^{\varepsilon_{F\nu}} d\varepsilon \rho_\nu(\varepsilon) \\ &\stackrel{(2.8)}{=} \frac{1}{t_\nu} \int_{\varepsilon_{\min\nu} + C_\nu}^{\varepsilon_{F\nu}} d\varepsilon \tilde{\rho}\left(\frac{\varepsilon - C_\nu}{t_\nu}\right) \\ \text{Subst. } \hat{\varepsilon} &= \frac{1}{t_\nu} (\varepsilon - C_\nu) \\ &= \int_{\frac{1}{t_\nu} \varepsilon_{\min\nu}}^{\frac{1}{t_\nu} (\varepsilon_{F\nu} - C_\nu)} d\hat{\varepsilon} \tilde{\rho}(\hat{\varepsilon}) \end{aligned}$$

## 2 Definition of the model system

For the case  $m = 0$  we can write this (using the relation  $\frac{1}{t_\nu}(\varepsilon_{\text{F}}^0 - C_\nu) \stackrel{(2.6)}{=} \tilde{\varepsilon}_{\text{F}}^0$  and the definition of  $\tilde{\varepsilon}_{\text{min}}$  (2.7)) as:

$$n_\nu^0 = \frac{n}{2} = \int_{\tilde{\varepsilon}_{\text{min}}}^{\tilde{\varepsilon}_{\text{F}}^0} d\varepsilon \tilde{\rho}(\varepsilon). \quad (2.9)$$

We are now interested in obtaining – in analogy to  $\tilde{\rho}$  and  $\tilde{\varepsilon}_{\text{F}}^0$  – a spin-independent expression  $\tilde{\varepsilon}^0 \equiv \tilde{\tilde{\varepsilon}}^0$  for the kinetic energy of a band:

$$\begin{aligned} \bar{\varepsilon}_\nu^0 &= \int_{\varepsilon_{\text{min}\nu} + C_\nu}^{\varepsilon_{\text{F}\nu}^0} d\varepsilon \rho_\nu(\varepsilon) \varepsilon \\ \text{Subst. as in (2)} \quad \hat{\varepsilon} &= \frac{1}{t_\nu}(\varepsilon - C_\nu) \\ &\stackrel{(2.6)}{=} \int_{\tilde{\varepsilon}_{\text{min}}}^{\tilde{\varepsilon}_{\text{F}}^0} d\hat{\varepsilon} \tilde{\rho}(\hat{\varepsilon})(t_\nu \hat{\varepsilon} + C_\nu) \\ &\stackrel{(2.9)}{=} t_\nu \underbrace{\int_{\tilde{\varepsilon}_{\text{min}}}^{\tilde{\varepsilon}_{\text{F}}^0} d\hat{\varepsilon} \tilde{\rho}(\hat{\varepsilon}) \hat{\varepsilon}}_{=: \tilde{\varepsilon}^0} + \frac{n}{2} C_\nu \end{aligned}$$

Finally we write this definition and the result properly:

$$\tilde{\varepsilon}^0 := \int_{\tilde{\varepsilon}_{\text{min}}}^{\tilde{\varepsilon}_{\text{F}}^0} d\varepsilon \tilde{\rho}(\varepsilon) \varepsilon, \quad (2.10)$$

$$\bar{\varepsilon}_\nu^0 = t_\nu \tilde{\varepsilon}^0 + \frac{n}{2} C_\nu. \quad (2.11)$$

The reason why we put so much effort in the calculation of the band-independent expressions  $\tilde{\rho}$ ,  $\tilde{\varepsilon}_{\text{F}}^0$  and  $\tilde{\varepsilon}^0$  is, that we will later want to describe the system in its direct dependence on  $(t_1 - t_2)$ .



### 3 Analytical results within the Hartree-Fock approximation

We start with the HFA energy expectation value (1.13) of the Hubbard model. Writing it using the DOS gives:

$$E_{\text{HF}} = \sum_{\nu} \bar{\varepsilon}_{\nu} + U n_1 n_2 \stackrel{(2.1)}{=} \sum_{\nu} \bar{\varepsilon}_{\nu} + \frac{U}{4} (n^2 - m^2). \quad (3.1)$$

The kinetic and the interaction term in (3.1) behave differently w.r.t. a change in  $m$ . The first has a positive derivation w.r.t.  $m$  as a higher orbital polarization corresponds to a state in which the movement of electrons is restricted. It is clear that this localization increases the kinetic energy of the electrons.

The competing effect is reflected in the interaction term which gets smaller for increasing  $m$ . This becomes mathematically obvious by looking at (3.1):  $E_{\text{int}} \propto -m^2$ , and has its deeper explanation in the fact that in HFA double occupancy can only be reduced by an increased polarization (whereas in a real correlated state there are more subtle ways to do so). This effect is the origin of the high overestimation of the fully polarized ferromagnetic phase in HFA.

In this work we are not interested in the known tendency to fully polarize ( $m = n$ ), but investigate if we can find an extremum  $m^* \neq 0$ , but close to 0. The general strategy (also for the next chapter) will be to expand  $E_{\text{HF}}$  (and later  $E_{\text{G}}$ ) – in the following just called  $E$  – at  $m = 0$ . We will first check if there is an extremum at  $m = 0$  by evaluating the first derivative. If there is one we will then analyze if it is a minimum or a maximum, if there is none we will identify the position of the minimum with the help of the second derivative. The expansion is:

$$E = E|_{m=0} + \left. \frac{dE}{dm} \right|_{m=0} m + \left. \frac{1}{2} \frac{d^2E}{dm^2} \right|_{m=0} m^2 + O(m^3). \quad (3.2)$$

We will need the following relations:

$$\frac{d\bar{\varepsilon}_{\nu}}{dm} = \int_{-\infty}^{\varepsilon_{\text{F}\nu}} d\varepsilon \rho_{\nu}(\varepsilon) \varepsilon = \rho_{\nu}(\varepsilon_{\text{F}\nu}) \varepsilon_{\text{F}\nu} \frac{d\varepsilon_{\text{F}\nu}}{dm}. \quad (3.3)$$

### 3 Analytical results within the Hartree-Fock approximation

Furthermore we have:

$$n_\nu = \int_{-\infty}^{\varepsilon_{F\nu}} d\varepsilon \rho_\nu(\varepsilon) \Rightarrow \frac{dn_\nu}{dm} = \rho_\nu(\varepsilon_{F\nu}) \frac{d\varepsilon_{F\nu}}{dm} \quad (3.4)$$

$$n_{1/2} = \frac{n \pm m}{2} \Rightarrow \frac{dn_{1/2}}{dm} = \pm \frac{1}{2}$$

$$\Rightarrow \frac{d\varepsilon_{F1/2}}{dm} = \pm \frac{1}{2 \rho_{1/2}(\varepsilon_{F1/2})}. \quad (3.5)$$

We arrive at:

$$\frac{d\bar{\varepsilon}_{1/2}}{dm} = \pm \frac{1}{2} \varepsilon_{F1/2} \quad (3.6)$$

$$\frac{d^2\bar{\varepsilon}_{1/2}}{d^2m} \stackrel{(3.5)}{=} \frac{1}{4 \rho_{1/2}(\varepsilon_{F1/2})}. \quad (3.7)$$

Now back to the expansion. It is clear that if the constant factor  $\left. \frac{dE}{dm} \right|_{m=0}$  is zero, one will find the extremum at  $m = 0$ . We get:

$$\begin{aligned} \left. \frac{dE}{dm} \right|_{m=0} &= \sum_\nu \left. \frac{d\bar{\varepsilon}_\nu}{dm} \right|_{m=0} + \frac{U}{4} \left. \frac{d}{dm} (n^2 - m^2) \right|_{m=0} \\ &\stackrel{(3.6)}{=} \underbrace{\frac{1}{2} (\varepsilon_{F1} - \varepsilon_{F2})}_{\stackrel{(2.5)}{=} 0} \Big|_{m=0} + \frac{U}{4} (-2m) \Big|_{m=0} = 0. \end{aligned} \quad (3.8)$$

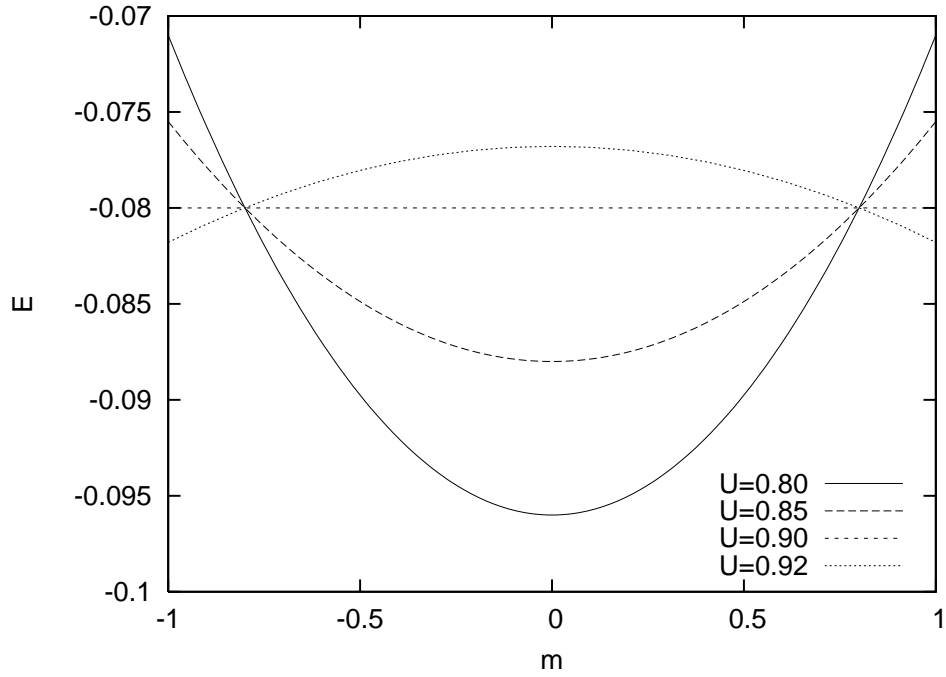
We now can state that the HFA – no matter which density of states we insert – always yields an extremum at  $m=0$ . It remains to check whether this is a minimum:

$$\begin{aligned} \left. \frac{d^2E}{dm^2} \right|_{m=0} &= \sum_\nu \left. \frac{d^2\bar{\varepsilon}_\nu}{d^2m} \right|_{m=0} + \frac{U}{4} \left. \frac{d}{dm} (-2m) \right|_{m=0} \\ &= \left( \frac{1}{4 \rho_1(\varepsilon_{F1})} + \frac{1}{4 \rho_2(\varepsilon_{F2})} \right) \Big|_{m=0} - \frac{U}{2} \end{aligned} \quad (3.9)$$

The second derivative is greater than zero if:

$$U < \frac{1}{2} \left( \frac{1}{\rho_1(\varepsilon_F)} + \frac{1}{\rho_2(\varepsilon_F)} \right) =: U_c, \quad (3.10)$$

i.e. we get a minimum provided the interaction is not too strong. If the interaction constant is bigger than a critical value  $U_c$ , one finds a maximum at  $m = 0$  (see Fig. 3.1).



**Figure 3.1:** Expectation value for the energy within the HFA. The parabola changes its sign for  $U = 0.90 \equiv U_c$ .

It is clear that for  $U > U_c$  the stable state of the system is at  $m = \pm n$  (none of the two possibilities is more likely to occur) and no longer in an unpolarized state. This effect is called Stoner instability.

### *3 Analytical results within the Hartree-Fock approximation*

## 4 Analytical results within the Gutzwiller approximation

The question is again, if the system – this time analyzed using the results of the Gutzwiller approximation – will be stable in a state with  $m = m^* \neq 0$  where  $m^*$  is small. We apply the same strategy as in the chapter before: expanding the energy expectation value at  $m = 0$ . First we give necessary conditions for the existence of the minimum. Second we evaluate its location, i.e. the magnitude of orbital polarization. All calculations were done for  $n \leq 1$ .

### 4.1 Conditions for orbital order

We start with (1.18) which is now analyzed for the investigated model. We can simplify the expression (1.18) by applying (2.3) and the consecutive equations. This gives us:  $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}1} = 0$  and  $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}2} = LC_2$ . If we now rewrite the remaining terms with the DOS expressions we get:

$$E(m, d) = \sum_{\nu} q_{\nu} \bar{\epsilon}_{\nu} + (1 - q_2) n_2 C_2 + Ud. \quad (4.1)$$

We have set  $E_G = E(m, d)$  where – in contrast to chapter 3 – a second variational parameter  $d$  occurs which can be traced back already to the GWF (see the introduction).

Minimizing has therefore to be done with respect to two variables. We will tackle the problem by first evaluating the condition for an extremum w.r.t. the second parameter  $d$

$$\left. \frac{\partial E}{\partial d} \right|_{m, d} = 0 \Rightarrow d = d^*(m), \quad (4.2)$$

and taking this as a constraint for the evaluation w.r.t.  $m$ .

Again we want to expand the energy at  $m = 0$ . We therefore need:

$$\left. \frac{dE}{dm} \right|_{m=0} = \left. \frac{\partial E}{\partial m} \right|_{m=0, d=d^*(0)} + \underbrace{\left. \frac{\partial E}{\partial d} \right|_{m=0, d=d^*(0)}}_{\stackrel{(4.2)}{=} 0} \left. \frac{\partial d^*}{\partial m} \right|_{m=0}. \quad (4.3)$$

In the further course of the work the common alternative notation for a partial derivative

#### 4 Analytical results within the Gutzwiller approximation

$f_x \equiv \frac{\partial f}{\partial x}$  will be frequently used (and the superscript  $0$  still indicates:  $f^0 := f|_{m=0}$ ).

With condition (4.2) we differentiate (4.1):

$$\frac{dE}{dm} \stackrel{(4.2)}{=} \sum_{\nu} \left( \frac{\partial q_{\nu}}{\partial m} \bar{\varepsilon}_{\nu} + q_{\nu} \frac{\partial \bar{\varepsilon}_{\nu}}{\partial m} \right) + \left( -\frac{\partial q_2}{\partial m} n_2 C_2 + (1 - q_2) \frac{\partial n_2}{\partial m} C_2 \right). \quad (4.4)$$

We need the derivatives at  $m = 0$ . It is therefore enough to give:

$$\left. \frac{\partial q_{1/2}}{\partial m} \right|_{m=0} = \mp 2(n-1) \frac{\left( 8d^2 + 4d - 8dn + n^2 - 4(n-2d)\sqrt{(1-n+d)d} \right)}{(n-2)^2 n^2} \quad (4.5)$$

where we used the relation  $n - 2d \geq 0$  which holds, as:

$$0 \leq \frac{1}{L} \sum_i \langle (\hat{n}_{i1} - \hat{n}_{i2})^2 \rangle = \frac{1}{L} \sum_i \langle \hat{n}_{i1}^2 + \hat{n}_{i2}^2 - \hat{n}_{i1} \hat{n}_{i2} \rangle = \frac{1}{L} \sum_i \langle \hat{n}_{i1} + \hat{n}_{i2} - \hat{n}_{i1} \hat{n}_{i2} \rangle = n - 2d.$$

All other derivatives in (4.4) have already been evaluated in chapter 3. We define in particular:  $q^0 := q_{\nu}|_{m=0}$ ,  $\mp q_m^0 := \left. \frac{\partial q_{1/2}}{\partial m} \right|_{m=0}$  and insert (3.4) and (3.6) in (4.5):

$$\begin{aligned} \left. \frac{dE}{dm} \right|_{m=0} &= q_m^0 (-\bar{\varepsilon}_1^0 + \bar{\varepsilon}_2^0) + \frac{q^0}{2} (\varepsilon_{F1}^0 - \varepsilon_{F2}^0) + \left( -q_m^0 \frac{n}{2} - (1 - q^0) \frac{1}{2} \right) C_2 \\ &\stackrel{(2.5)}{=} q_m^0 \left( \underbrace{\bar{\varepsilon}_2^0 - \bar{\varepsilon}_1^0}_{\stackrel{(2.11)}{=} (t_2 - t_1) \bar{\varepsilon}^0 + \frac{n}{2} C_2} - \frac{C_2}{2} \underbrace{\left( n + \frac{1 - q^0}{q_m^0} \right)}_{= \frac{n^2}{2(n-1)}} \right) \end{aligned} \quad (4.6)$$

With  $C_2 \stackrel{(2.6)}{=} (t_1 - t_2) \bar{\varepsilon}_F^0$  we can summarize the condition for an extremum – which we assume to be again a minimum for a not so strong interaction constant  $U$  – at  $m = 0$  to:

$$\boxed{(t_1 - t_2) q_m^0 \left( -\bar{\varepsilon}^0 + \bar{\varepsilon}_F^0 \frac{n(n-2)}{4(n-1)} \right) = 0} \quad (4.7)$$

It is clear that this will in general not hold, as the bracket in (4.7) can – using (2.10) – be written as the following integral equation for  $\bar{\varepsilon}_F^0$  which is not fulfilled in general:

$$\int_{\bar{\varepsilon}_{\min}}^{\bar{\varepsilon}_F^0} d\varepsilon \tilde{\rho}(\varepsilon) \varepsilon - \bar{\varepsilon}_F^0 \frac{n(n-2)}{4(n-1)} = 0. \quad (4.8)$$

We can immediately give exceptions: There are (at least) three independent situations – apart from singular choices of  $n$  which lead to a satisfied condition (4.8) – each of which is sufficient for (4.7) to hold:

$$\boxed{\text{Case 1: } U = 0 \quad \text{Case 2: } n = 1 \quad \text{Case 3: } \tilde{\rho}(\varepsilon) = \text{const}}$$

#### 4.1 Conditions for orbital order

To prove this, we need the explicit form of (4.2) for  $m = 0$ . We define  $q_d^0 := \left. \frac{\partial q_\nu}{\partial d} \right|_{m=0}$  and get:

$$\left. \frac{\partial E}{\partial d} \right|_{m=0, d=d^*(0)} = 0 \quad \Leftrightarrow \quad q_d^0 \underbrace{\left( \tilde{\varepsilon}_1^0 + \tilde{\varepsilon}_2^0 - \frac{n}{2} C_2 \right)}_{\stackrel{(2.11)}{=} (t_1 + t_2) \tilde{\varepsilon}^0} + U = 0 \quad (4.9)$$

where

$$q_d^0 = - \frac{8 \left( \sqrt{d \left( \frac{n}{2} - d \right)} + \sqrt{(1 - n + d) \left( \frac{n}{2} - d \right)} \right)}{(n - 2)n \sqrt{2d(n - 2d)(d - n + 1)}} \left( \sqrt{(1 - n + d) \left( \frac{n}{2} - 2d \right)} + \sqrt{d} \left( -2d + 3 \frac{n}{2} - 1 \right) \right) \quad (4.10)$$

**Proof Case 1:**  $U = 0$

If  $U = 0$ , it follows from (4.9) that  $q_d^0(d) \stackrel{!}{=} 0$  which yields the uncorrelated expectation value  $d = \frac{n^2}{4}$  for the double occupancy. This is easily checked by considering the second factor in (4.10):

$$d = \frac{n^2}{4} \stackrel{(4.10)}{\Rightarrow} \underbrace{\sqrt{\left( \frac{n^2}{4} - n + 1 \right)}}_{\stackrel{n \leq 2}{=} 1 - \frac{n}{2}} \underbrace{\left( \frac{n}{2} - 2 \frac{n^2}{4} \right)}_{\frac{n}{2}(1 - n)} + \frac{n}{2} \underbrace{\left( -2 \frac{n^2}{4} + 3 \frac{n}{2} - 1 \right)}_{-(1 - n) \left( 1 - \frac{n}{2} \right)} = 0 \quad (4.11)$$

It is similarly simple to check  $q_m^0 \left( d = \frac{n^2}{4} \right) = 0$  by evaluating (4.5). Eq.(4.7) then follows directly.

**Proof Case 2:**  $n = 1$

Rewrite (4.7):

$$(t_1 - t_2) \frac{q_m^0}{n - 1} \left( -(n - 1) \tilde{\varepsilon}^0 + \tilde{\varepsilon}_F^0 \frac{n(n - 2)}{4} \right) = 0 \quad (4.12)$$

The terms in the bracket give zero for  $n = 1$  (as  $\tilde{\varepsilon}_F^0 = 0$ ). The term  $\frac{q_m^0}{n - 1}$  is finite, which is obvious when comparing it with (4.5).

**Proof Case 3:**  $\tilde{\rho}(\varepsilon) = \text{const}$

We evaluate (2.9) for the normalized DOS  $\rho_\nu = \frac{1}{t_\nu} \Rightarrow \tilde{\rho}(\varepsilon) = 1$ , i.e.  $\tilde{\varepsilon}_{\min\nu} = -\frac{1}{2}$  and get:

$$\frac{n}{2} = \int_{-\frac{1}{2}}^{\tilde{\varepsilon}_F^0} d\varepsilon \quad \Leftrightarrow \quad \tilde{\varepsilon}_F^0 = \frac{n - 1}{2}. \quad (4.13)$$

## 4 Analytical results within the Gutzwiller approximation

With (2.10) we get:

$$\tilde{\varepsilon}^0 = \int_{-\frac{1}{2}}^{\frac{n-1}{2}} d\varepsilon \varepsilon = \frac{1}{8}n(n-2) \quad (4.14)$$

Inserting these two results for  $\tilde{\varepsilon}_F^0$  and  $\tilde{\varepsilon}^0$  in (4.12) immediately shows that (4.7) holds.

## 4.2 Magnitude of the orbital polarization

### 4.2.1 Formal evaluation for the case of not too strong $U$

Until now we did not check whether we will indeed get a minimum and not a maximum for  $m^*$ . This check could in principle be done by analyzing the sign of the complicated second derivative of  $E$ . For now we will omit this check and assume that we deal with a minimum. Furthermore we do not allow  $U$  to get so big, that it could induce the fully polarized state, as we are not interested in the Stoner instability. In the numerical part of the work, chapter 5, one will see that these assumptions are justified.

Let's consider the expansion of the energy (3.2) again. We assume that the minimum is close enough to  $m = 0$ , that we can take the parabola as a good approximation of the actual function. If that is the case, we can immediately give the position of the minimum:

$$m^* = -\frac{\left.\frac{dE}{dm}\right|_{m=0}}{\left.\frac{d^2E}{dm^2}\right|_{m=0}} + O(m^*)^3. \quad (4.15)$$

This was achieved by completing the square:  $a m^2 + b m = a \left(m + \frac{b}{2a}\right)^2 - \frac{b^2}{4a^2} \Rightarrow m^* = -\frac{b}{2a}$  where  $a = \frac{1}{2} \left.\frac{d^2E}{dm^2}\right|_{m=0}$  and  $b = \left.\frac{dE}{dm}\right|_{m=0}$ .

We evaluate the second derivative of  $E$  w.r.t.  $m$ :

$$\frac{d^2E}{dm^2} = E_{mm} + 2E_{md} \frac{\partial d}{\partial m} + E_d \frac{\partial^2 d}{\partial m^2} + E_{dd} \left(\frac{\partial d}{\partial m}\right)^2 \quad (4.16)$$

and consider it at  $m = 0$  assuming condition (4.2) to be fulfilled:

$$\left.\frac{d^2E}{dm^2}\right|_{m=0, d=d^*(0)} \stackrel{(4.2)}{=} E_{mm}|_{0, d^*(0)} + 2 E_{md}|_{0, d^*(0)} \left.\frac{\partial d^*}{\partial m}\right|_0 + E_{dd}|_{0, d^*(0)} \left(\left.\frac{\partial d^*}{\partial m}\right|_0\right)^2. \quad (4.17)$$

In the following the terms which appear in  $\left.\frac{dE}{dm}\right|_{m=0}$  and  $\left.\frac{d^2E}{dm^2}\right|_{m=0}$  are written down explicitly in a form that shows their direct dependence on  $t_1$  and  $t_2$ .

$E_m^0$  is just (4.6):

$$E_m^0 = (t_1 - t_2) q_m^0 \left(-\tilde{\varepsilon}^0 + \tilde{\varepsilon}_F^0 \frac{n(n-2)}{4(n-1)}\right). \quad (4.18)$$



## 4.2 Magnitude of the orbital polarization

Using  $\rho_\nu(\varepsilon_{\text{F}}^0) = \frac{1}{t_\nu} \tilde{\rho}(\tilde{\varepsilon}_{\text{F}}^0) =: \frac{1}{t_\nu} \tilde{\rho}^0$  we can evaluate  $E_{mm}^0$  starting from (4.4). We state that  $q_{\nu mm}|_{m=0} = q_{mm}^0$ . The result is:

$$E_{mm}^0 = (t_1 + t_2) \left( q_{mm}^0 \tilde{\varepsilon}^0 - q_m^0 \tilde{\varepsilon}_{\text{F}}^0 + \frac{1}{4} \frac{q^0}{\tilde{\rho}^0} \right). \quad (4.19)$$

$E_{md}^0$  formally follows immediately from (4.18):

$$E_{md}^0 = (t_1 - t_2) q_{md}^0 \left( -\tilde{\varepsilon}^0 + \tilde{\varepsilon}_{\text{F}}^0 \frac{n(n-2)}{4(n-1)} \right). \quad (4.20)$$

$E_{dd}^0$  follows directly from (4.9):

$$E_{dd}^0 = (t_1 + t_2) q_{dd}^0 \tilde{\varepsilon}^0. \quad (4.21)$$

To complete this, one has to give the explicit form of the derivatives of  $q$ .  $q_m^0$  and  $q_d^0$  have already been evaluated in (4.5) and (4.10). The remaining derivatives are listed below:

$$q_{mm}^0 = 4 \left( 16 \frac{d^2}{n^3} - 24 \frac{d^2}{n^2} + 12 \frac{d^2}{n} + 8 \frac{d}{n^3} - 28 \frac{d}{n^2} + 30 \frac{d}{n} - 12d + n - 1 \right. \\ \left. + (n-2d) \sqrt{(1-n+d)d} \left( -\frac{8}{n^3} + \frac{12}{n^2} - \frac{6}{n} + \frac{(n-2)^2}{n(n-2d)^2} \right) \right) \frac{1}{(n-2)^3} \quad (4.22a)$$

$$q_{md}^0 = 4(n-1)(n-2d) \left( 2\sqrt{(1-n+d)d} (1-2(n-2d)) \right. \\ \left. + 8d^2 + n^2 - n + 2d(4n-3) \right) \\ \times \frac{1}{(n-2)^2 n^2 (n-2d) \sqrt{(1-n+d)d}} \quad (4.22b)$$

$$q_{dd}^0 = \left( -32d^4 + 16(4n-3)d^3 + 16(d^2 + 4(n-1)d)(n-2d) \sqrt{(1-n+d)d} \right. \\ \left. + 12(n(4-3n) - 1)d^2 + 4(n-1)^2 n d + (n-1)^2 n^2 \right) \\ \times \frac{1}{(n-2)n(n-2d) \left( \sqrt{(1-n+d)d} \right)^3} \quad (4.22c)$$

where we again used the relation  $n-2d \geq 0$ .

The only term which remains to evaluate is  $\frac{\partial d^*}{\partial m} \Big|_{m=0}$ . To calculate it we would need the explicit or the inverse function of  $d^*(m)$ , both of which are hard to get from the constraint (4.2), as already the simplified equation (4.9) (there  $m$  equals zero) is analytically solvable not without great effort. Additionally the result of this calculation is too complicated to provide any meaningful information. We therefore have to think about an approximation of the constraint. It seems advisable for this procedure to make use of the fact that our derivation of the minimum  $m^*$  is correct only in quadratic order in  $m$  (Taylor expansion), so that if we keep the order  $m^2$ , we will not lose any accuracy.

### Approximating the constraint w.r.t. $m$

We have to get  $\frac{\partial d^*}{\partial m}|_{m=0}$  from the constraint (4.2) for general  $m$ . We write it down explicitly (we already did it for the special case  $m = 0$  in (4.9)):

$$\frac{\partial E}{\partial d}\Big|_{m, d^*(m)} = 0 \Leftrightarrow \underbrace{q_{1d}\bar{\varepsilon}_1 + q_{2d}\left(\bar{\varepsilon}_2 - \frac{n-m}{2}C_2\right)}_{=: f(m, d)} + U = 0 \quad (4.23)$$

where we defined a function  $f(m, d)$  just to keep the notation bearable.

We expand it w.r.t.  $m$ :

$$f(m, d) = f(0, d) + f_m(0, d)m + \frac{1}{2}f_{mm}(0, d)m^2 + O(m^3) \quad (4.24)$$

We can now easily get  $m(d)$  as we only deal with a quadratic equation:

$$m(d) = \frac{-f_m^0(d) + \sqrt{(f_m^0(d))^2 - 2f_{mm}^0(d)(f^0(d) + U)}}{f_{mm}^0(d)} \quad (4.25)$$

where we chose the "+" solution of the quadratic formula being the solution which reflects the behavior in linear order.

We get  $\frac{\partial d^*}{\partial m}|_{m=0}$  by applying the rule for the derivative of an inverse function:

$$\frac{\partial d^*}{\partial m}\Big|_{m=0} = \frac{1}{\frac{\partial m}{\partial d}\Big|_{d=d^*(m=0)}}. \quad (4.26)$$

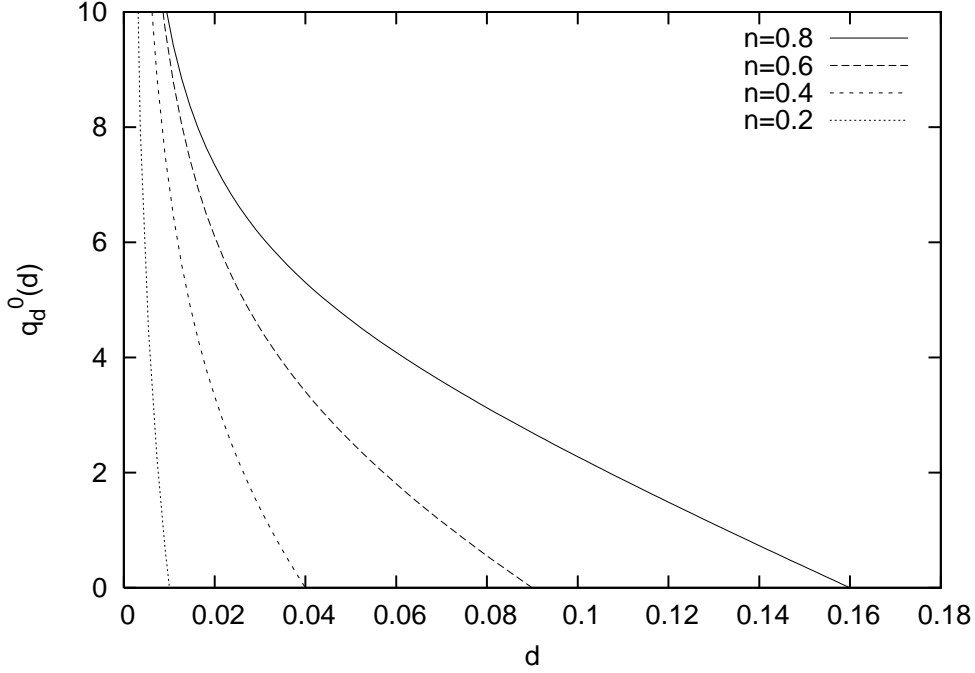
With that we have formally solved the problem by finding the minimum. The obstacle which makes it hard to get the final explicit solution is to evaluate the value of  $d^*(m = 0)$  in (4.26). This can in principal be done by solving (4.9) like we did it in Proof 1 before, but this time for  $U \neq 0$ :

$$(4.9) \Rightarrow q_d^0(d) \stackrel{!}{=} -\frac{U}{(t_1 + t_2)\bar{\varepsilon}^0}, \quad (4.27)$$

where  $q_d^0(d)$  is given by (4.10).

With that we have the strategy for a numerical solution of the problem. The latter will not constitute a problem, as  $q_d^0$  is a well behaved function in the interval of interest. In Fig. 4.1 this becomes obvious. There we also see that  $q_d^0(\frac{n^2}{4}) = 0$  (have a look at the intersections with the  $d$ -axis:  $\frac{n^2}{4} = 0.16$  for  $n = 0.8, \dots$ ).

The explicit numerical solution will be done for the Bethe lattice in chapter 5. We will now not further investigate the general case but restrict ourselves on the evaluation for small  $U$ .



**Figure 4.1:** The discontinuity at the Fermi edge of the momentum distribution (for  $m = 0$ )  $q_d^0$  is a smooth function. It is plotted for different  $n$ . The intersections with the  $d$ -axis are found at  $\frac{n^2}{4}$ .

#### 4.2.2 Explicit results for a small interaction constant $U$

Now we want to gain explicit results for the behavior of  $m^*$ . The problem in the section before was, that the dependence of the constraint on  $d$  was too complicated to yield meaningful results. Therefore we expand it also w.r.t. to  $d$ .

##### Approximating the constraint w.r.t. $d$

We again look at Eq.(4.23) and expand it w.r.t.  $d$ . As we approximate for small  $U$ , we expand at the  $U = 0$  value for the double occupancy  $d = \frac{n^2}{4}$ . For convenience in the notation we introduce the variable  $\delta$  (being the negative difference of the actual and the  $U = 0$  value of  $d$ ):

$$\delta := d - \frac{n^2}{4}. \quad (4.28)$$

With that we get (in analogy to (4.24)):

$$f(m, d) = f(0, \frac{n^2}{4}) + f_m(0, \frac{n^2}{4}) m + \frac{1}{2} f_{mm}(0, \frac{n^2}{4}) m^2 + f_d(0, \frac{n^2}{4}) \delta + O(m^3, \delta^2, m \delta) \quad (4.29)$$

We dropped the  $O(m \delta)$  term as it would exceed the linear order in  $\delta$ .

We recognize by comparison with (4.9) that we already can formally write down two of

#### 4 Analytical results within the Gutzwiller approximation

the terms in (4.29):

$$f(0, \frac{n^2}{4}) = q_d^0(\frac{n^2}{4}) (t_1 + t_2) \tilde{\varepsilon}^0 \quad (4.30a)$$

$$f_d(0, \frac{n^2}{4}) = q_{dd}^0(\frac{n^2}{4}) (t_1 + t_2) \tilde{\varepsilon}^0 \quad (4.30b)$$

We get the  $m$  terms by explicit differentiation. Again we make use of our former definition:  $q_{1/2m}|_{m=0} = \mp q_m^0 \Rightarrow q_{1/2md}|_{m=0} = \mp q_{md}^0 = \mp q_{dm}^0$ , and get with an analog relation for the second derivative  $q_{\nu mm}|_{m=0}$  ( $q_{\nu mmd}|_{m=0} = q_{dmm}^0$ ):

$$\begin{aligned} f_m(0, d) &= q_{1dm}(0, \frac{n^2}{4}) \bar{\varepsilon}_1^0 + q_{2dm}(0, \frac{n^2}{4}) (\bar{\varepsilon}_2 - \frac{n-m}{2} C_2)|_{m=0} + q_{2d}(0, \frac{n^2}{4}) \frac{1}{2} C_2 \\ &= -q_{dm}^0(\frac{n^2}{4}) (t_1 - t_2) \tilde{\varepsilon}^0 + q_d^0(\frac{n^2}{4}) \frac{1}{2} C_2 \end{aligned} \quad (4.31a)$$

$$f_{mm}(0, d) = q_{dmm}^0(\frac{n^2}{4}) (t_1 + t_2) \tilde{\varepsilon}^0 + q_{dm}^0(\frac{n^2}{4}) C_2 \quad (4.31b)$$

This is completed by the following results for the  $q$  terms:

$$\begin{aligned} q_d^0(\frac{n^2}{4}) &= 0 \\ q_{dd}^0(\frac{n^2}{4}) &= \frac{32}{(n-2)^3 n^3} \\ q_{dm}^0(\frac{n^2}{4}) &= 0 \\ q_{dmm}^0(\frac{n^2}{4}) &= \frac{16}{(n-2)^3 n^3} \end{aligned} \quad (4.32)$$

We are now able to write down the approximated constraint (4.23) (by inserting (4.29) in it) being correct for small  $m$  and small  $U$ :

$$\boxed{\frac{8}{(n-2)^3 n^3} (t_1 + t_2) \tilde{\varepsilon}^0 m^2 + \frac{32}{(n-2)^3 n^3} (t_1 + t_2) \tilde{\varepsilon}^0 (d - \frac{n^2}{4}) + U = 0} \quad (4.33)$$

Now we easily get  $\frac{\partial d^*}{\partial m}|_{m=0}$ . We isolate  $d$  and differentiate w.r.t.  $m$ :

$$\frac{\partial d^*}{\partial m} \Big|_{m=0} = -8 m|_{m=0} = 0 \quad (4.34)$$

With that result the minimum  $m^*$  is given in a very simple form (see (4.15) and the following equations):

$$m^* = -\frac{E_m^0}{E_{mm}^0} = -\frac{(t_1 - t_2) q_m^0 \left( -\tilde{\varepsilon}^0 + \tilde{\varepsilon}_F^0 \frac{n(n-2)}{4(n-1)} \right)}{(t_1 + t_2) \left( q_{dmm}^0 \tilde{\varepsilon}^0 - q_m^0 \tilde{\varepsilon}_F^0 + \frac{1}{4} \frac{q^0}{\rho^0} \right)} \quad (4.35)$$

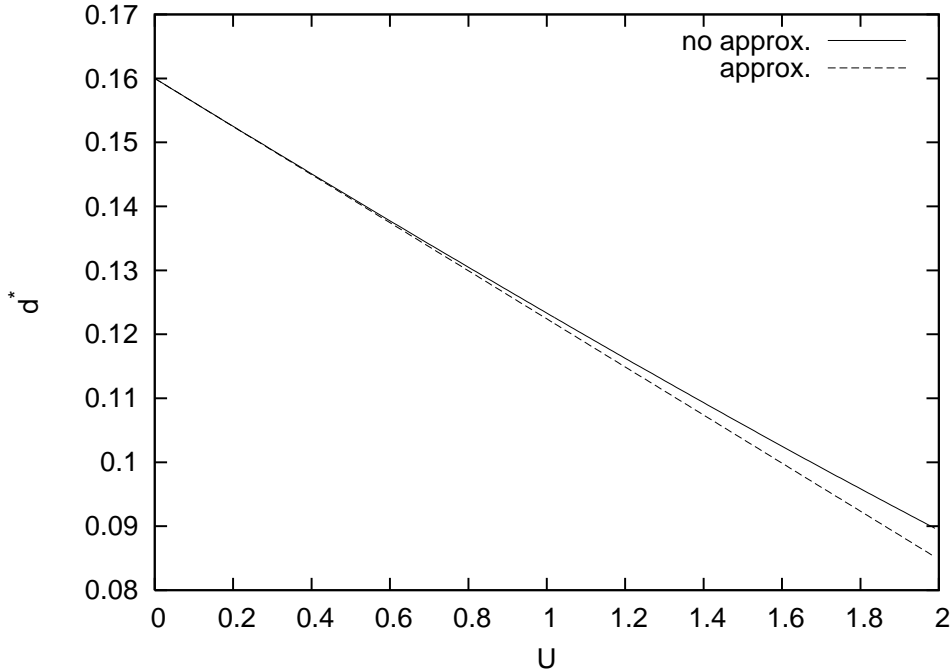
We want to learn something about the general behavior of  $m^*$ , first w.r.t. to the interaction constant  $U$  and second w.r.t. to the anisotropy  $t_1 - t_2$ . We keep in mind that the expression (4.35) still depends on  $d$  in a complicated way (in the  $q$ -terms).

### Interaction $U$

How does  $m^*$  depend on  $U$ ? Interaction appears in the expression for  $m^*$  nowhere else than in the  $q$  terms in form of the  $U$ -dependent double occupancy  $d$ . That is clear as the GA yields not more than a constant approximation of the momentum space occupancy inside and outside the  $U = 0$  Fermi surface. The double occupancy  $d$  gets its dependence on  $U$  from the constraint. The Taylor ansatz demands the evaluation of the latter at  $m = 0$ , so that we can write the constraint within the approximation of small  $U$  in linear order (4.33) for  $m = 0$ :

$$\delta = d^* - \frac{n^2}{4} = -\frac{(n-2)^3 n^3}{32(t_1+t_2)\tilde{\varepsilon}^0} U \quad (4.36)$$

Expanding the minimum  $m^*$  w.r.t.  $d$  is now equivalent to expanding it w.r.t.  $U$  using that given relation. See Fig. 4.2 which compares this relation, i.e. the approximation of  $d^*$ , with the exact value of  $d^*$  (for the constraint corresponding to the semi-elliptic DOS).



**Figure 4.2:** The exact result for  $d^*$  compared with the the approximation (4.36).

Now we have to expand the  $q$  terms as these still are too complicated. We first consider the order up to which we have to expand. It is clear that the orbital order effect that

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we are investigating will be at least of order  $U^2$ , otherwise it would have emerged in the Hartree-Fock approximation, too. We are not interested in higher orders, as we treat small  $U$  anyway.

The question which then arises is why we did not expand to order  $U^2$  in (4.33), (4.36) respectively. In fact we will see that  $m^* \propto \delta^2$ . It is clear that if we expanded to quadratic order in (4.33) we would have gained a relation in (4.36) where  $\delta \propto AU^2 + BU$  where the prefactor  $B$  would be the same as in the linear order approximation we are making use of. As  $m^* \propto \delta^2$  all terms which include  $A$  would already be of order  $U^4$  that we do not want to consider. Therefore it is clear that the linear approximation in (4.36) is enough.

Another aspect is the accuracy with which one has to evaluate the single  $q$  terms. If the fraction which constitutes  $m^*$  looks like this:

$$\frac{C \delta^2}{D + E \delta} = \frac{C \delta^2}{D} (1 + O(\delta)), \quad (4.37)$$

we can state that - as long as there is a constant term in the denominator - we will not have to expand the other denominator terms to a higher than the constant order.

Keeping that in mind we look at the expansions of the  $q$  terms w.r.t. to  $\delta$ , again at the point  $(m = 0, d = \frac{n^2}{4})$ . The result (4.35) tells us that  $q_m^0$  is the only term which appears in the numerator and which we therefore have to expand up to second order. Evaluation (and application of the former results  $q_m^0(\frac{n^2}{4}) = 0$ ,  $q_{md}^0(\frac{n^2}{4}) = 0$ ,  $q_d^0(\frac{n^2}{4}) = 0$ ) yields:

$$\begin{aligned} q_m^0(d) &= q_m^0\left(\frac{n^2}{4}\right) + q_{md}^0\left(\frac{n^2}{4}\right) \delta + \frac{1}{2} q_{mdd}^0\left(\frac{n^2}{4}\right) \delta^2 + O(\delta^3) \\ &= \frac{32(n-1)}{(n-2)^4 n^4} \delta^2 + O(\delta)^3. \end{aligned} \quad (4.38)$$

And for the denominator terms:

$$\begin{aligned} q^0(d) &= q^0\left(\frac{n^2}{4}\right) + q_d^0\left(\frac{n^2}{4}\right) \delta + O(\delta^2) \\ &= 1 + O(\delta) \end{aligned} \quad (4.39a)$$

$$\begin{aligned} q_{mm}^0(d) &= q_{mm}^0\left(\frac{n^2}{4}\right) + q_{mmd}^0\left(\frac{n^2}{4}\right) \delta + O(\delta^2) \\ &= O(\delta). \end{aligned} \quad (4.39b)$$

With the insertion of these results in (4.35) we get:

$$m^* = - \frac{(t_1 - t_2) \frac{32(n-1)}{(2-n)^4 n^4} \delta^2 \left( -\tilde{\varepsilon}^0 + \tilde{\varepsilon}_F^0 \frac{n(n-2)}{4(n-1)} \right)}{(t_1 + t_2) \left( \frac{1}{4} \frac{1}{\rho^0} \right)}. \quad (4.40)$$

Finally, (4.36) leads to the explicit expression for  $m^*$  in the approximation of small  $U$

## 4.2 Magnitude of the orbital polarization

and small  $m$ :

$$m^* = \frac{(n-1)(n-2)^2 n^2}{8} \frac{t_1 - t_2}{t_1 + t_2} \tilde{\rho}^0 \left( \tilde{\varepsilon}^0 - \tilde{\varepsilon}_F^0 \frac{n(n-2)}{4(n-1)} \right) \left( \frac{U}{(t_1 + t_2) \tilde{\varepsilon}^0} \right)^2 \quad (4.41)$$

We keep in mind that  $t_1$ ,  $t_2$  and  $U$  are in units of energy and all quantities with a tilde are dimensionless so that  $m^*$  is unitless as it should be.

### Anisotropy $t_1 - t_2$

One now can immediately give the exact dependence of the approximate  $m^*$  on  $t_1$  and  $t_2$  by looking at (4.41):

$$m^* \propto \frac{t_1 - t_2}{t_1 + t_2}. \quad (4.42)$$

To consider it for a small difference  $t_1 - t_2$  we set  $t_1 \equiv 1$  (without loss of generality) and define  $\beta := t_1 - t_2 \equiv 1 - t_2$ . Now we can state that:

$$m^* \propto \frac{\beta}{2 - \beta} \stackrel{\beta \text{ small}}{=} \frac{1}{2} \beta (1 + O(\beta)). \quad (4.43)$$

We see that the dependence on the anisotropy is linear in first order, i.e. the position of the minimum – the strength of orbital order respectively – is proportional to the difference in the hopping constants, if this difference is small.

#### 4 *Analytical results within the Gutzwiller approximation*



## 5 Numerical results within the Gutzwiller approximation

In the following all analytic results will be looked at in terms of explicit numerical calculations for the elliptic DOS of the Bethe lattice:

$$\rho(\varepsilon) = \begin{cases} \frac{1}{2\pi t_\nu^2} \sqrt{4t_\nu^2 - (\varepsilon - C_\nu)^2} & \text{for } |\varepsilon - C_\nu| < 2t_\nu \\ 0 & \text{else.} \end{cases}$$

### 5.1 Plots of the energy $E$

Fig. 5.1 shows the relation between the energy expectation value and the orbital polarization  $m$  for different values of  $U$ . Here the calculations were done exactly (without applying any approximations) within the numerical accuracy. One sees that the polarization  $m^*$  which corresponds to the minimum of the energy has a greater value for greater  $U$ .

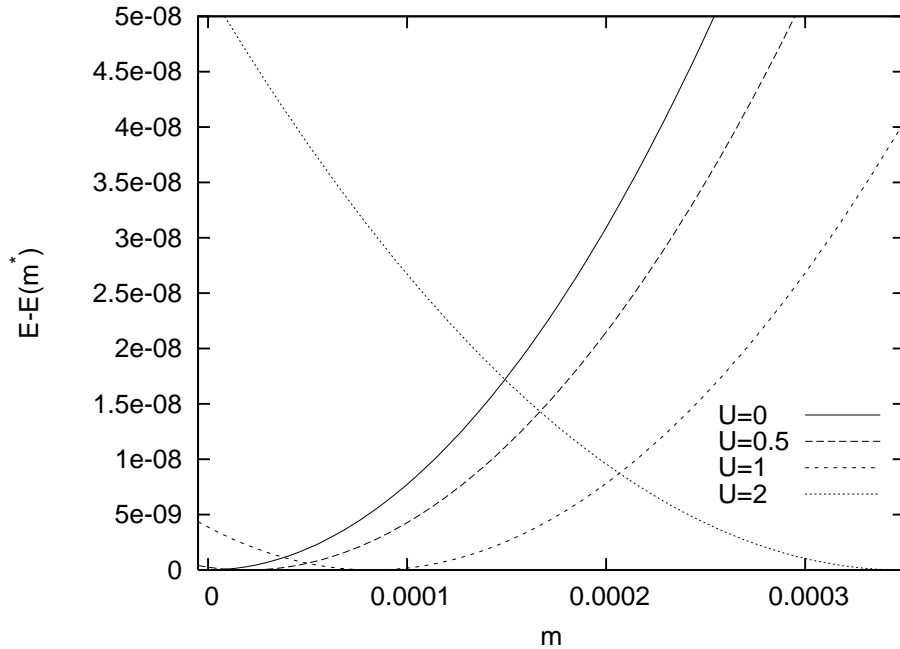


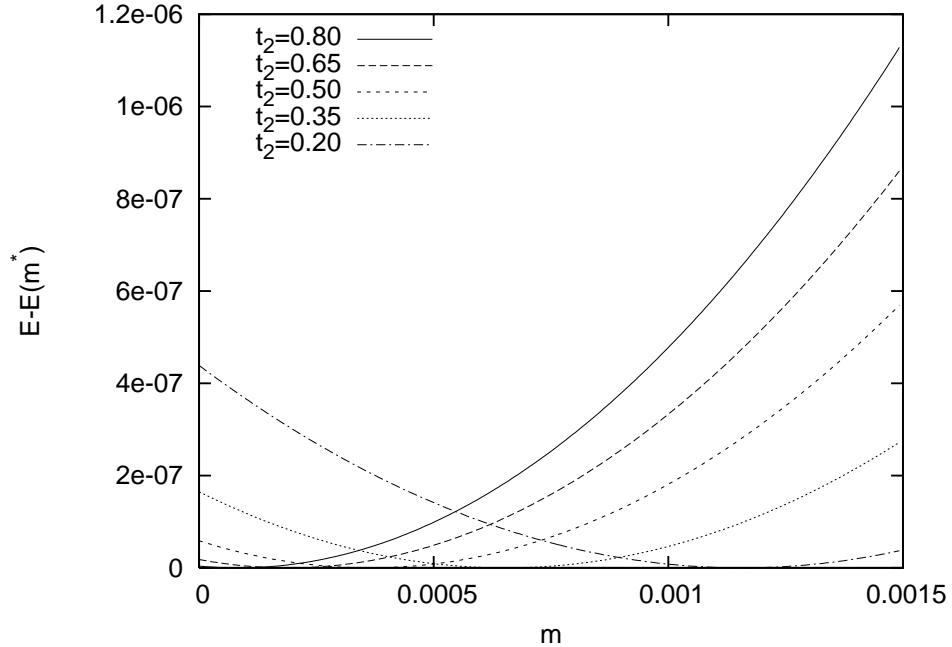
Figure 5.1: Parameters:  $n = 0.5$ ,  $t_1 = 1$ ,  $t_2 = 0.8$

## 5 Numerical results within the Gutzwiller approximation

The following tabular provides the numerical results for the location of the minima in the plot and compares them with the results achieved using the Taylor expansion in  $m$  (4.15) and those using the additional Taylor expansion (this time of the side condition) in  $U$  (4.41). As it was expected, both approximations yield meaningful results for small  $U$ . The steps between the values of  $U$  were chosen so that one can easily recognize the proportionality  $m^* \propto U^2$ . Below we will then see plots which show the dependence of  $m^*$  on  $U$  more clearly.

$m^*$	Plot (numerically exact)	approx. w.r.t. $m$	approx. w.r.t. $m$ and $U$
$U = 0$	0	0	0
$U = \frac{1}{2}$	0.00001875	0.00001958	0.00001821
$U = 1$	0.00008200	0.00008263	0.00007384
$U = 2$	0.00034875	0.00034200	0.00028567

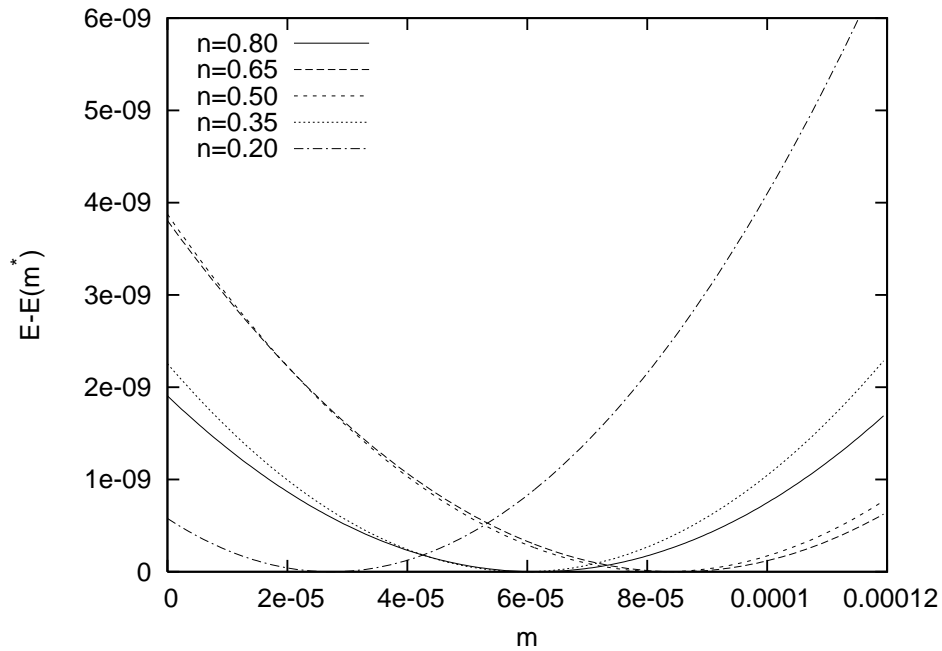
In plot Fig. 5.2 the unapproximated  $E$  is plotted versus  $m$  but this time for different hopping constants  $t_2$ . It therefore shows the dependence of  $E$  on  $t_1 - t_2$ . We state that the orbital order effect gets stronger for a growing difference  $t_1 - t_2$ . We will also compare this result in Fig. 5.7.



**Figure 5.2:** Parameters:  $n = 0.5$ ,  $U = 1$ ,  $t_1 = 1$

### 5.1 Plots of the energy $E$

In Fig. 5.3 one sees a last plot for the unapproximated  $E$ . This time for different  $n$ . One can state that the polarization is strongest in the interval  $[0.5, 0.8]$  ( $n = 0.65$  yields the greatest magnitude of  $m^*$  in the plot). This is discussed in terms of the approximated result in the context of Fig. 5.8.



**Figure 5.3:** Parameters:  $U = 1$ ,  $t_1 = 1$ ,  $t_2 = 0.8$

All these plots of the energy  $E$  confirm the assumptions that we indeed deal with a minimum (and not with a maximum) at  $m = m^*$  and that  $m^*$  has a small magnitude.

## 5.2 Plots of the orbital polarization $m^*$

The following pictures show the orbital polarization in its dependence on  $U$ . Plotted are the numerically exact results and the results calculated within the two approximations. There are three plots for  $n = 0.2$ ,  $n = 0.5$ ,  $n = 0.8$ . For all three values of  $n$  the exact results show a similar behavior and are – at least for small  $U$  – well approximated.

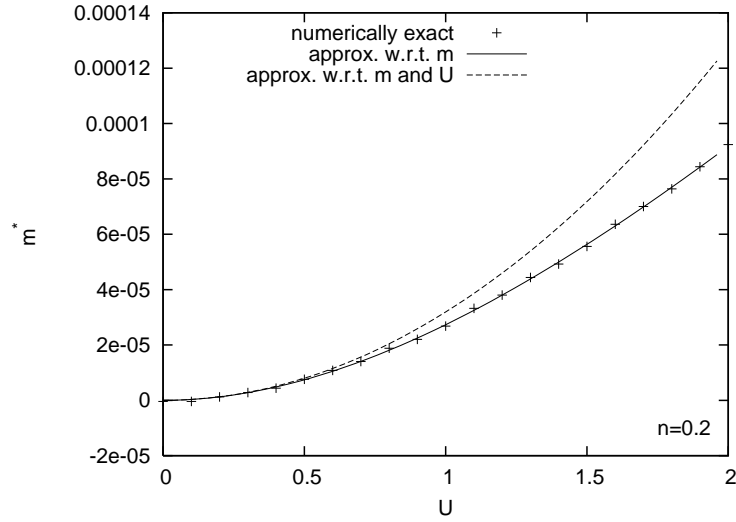


Figure 5.4: Parameters:  $n = 0.2$ ,  $t_1 = 1$ ,  $t_2 = 0.8$

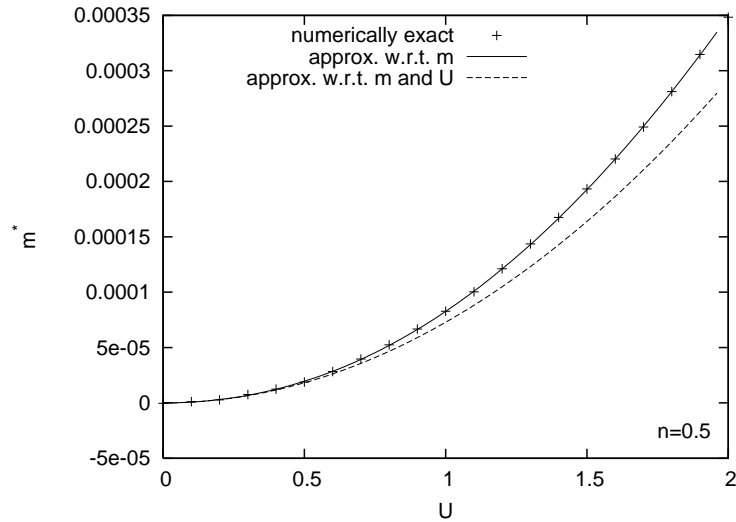
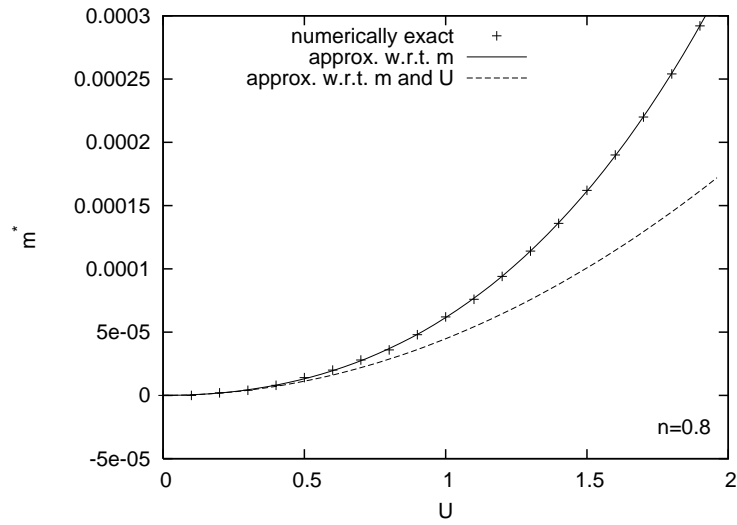


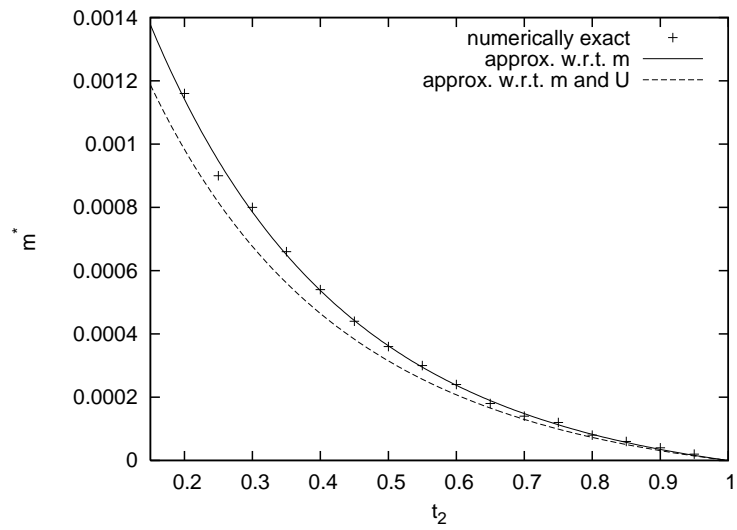
Figure 5.5: Parameters:  $n = 0.5$ ,  $t_1 = 1$ ,  $t_2 = 0.8$

5.2 Plots of the orbital polarization  $m^*$



**Figure 5.6:** Parameters:  $n = 0.8$ ,  $t_1 = 1$ ,  $t_2 = 0.8$

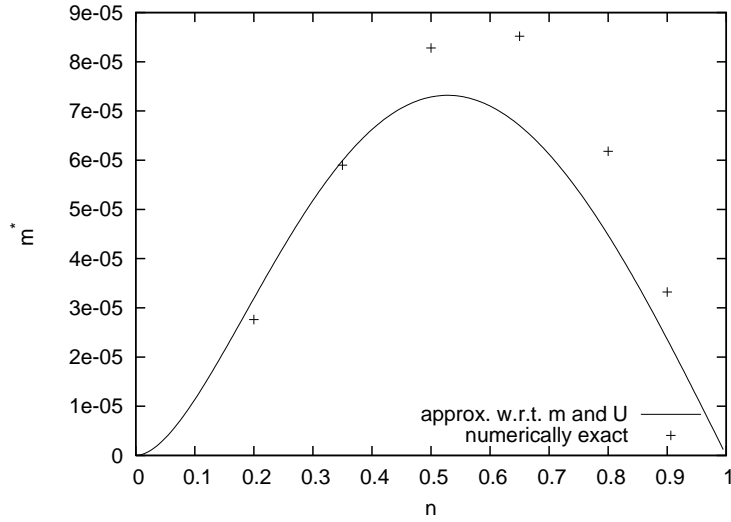
Fig. 5.7 now shows the dependence of  $m^*$  on  $t_2$ . We state once more that the position of the minimum grows with a growing difference  $t_1 - t_2$  (which corresponds to a shrinking  $t_2$ ).



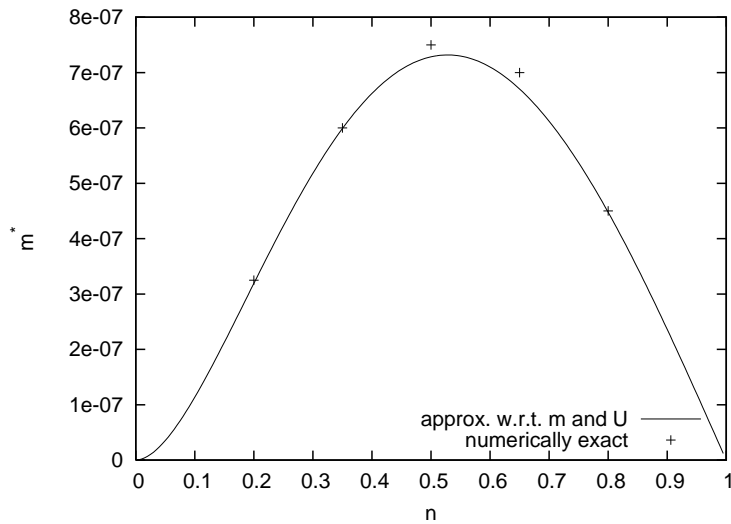
**Figure 5.7:** Parameters:  $n = 0.5$ ,  $U = 1$ ,  $t_1 = 1$

## 5 Numerical results within the Gutzwiller approximation

In the last pictures we plot the result for  $m^*$  (4.41) versus  $n$  for fixed  $U$ . The maximum can be found at  $n = 0.5$ . Looking at Fig. 5.8 we state that for  $U = 1$  the approximation is rough (the exact results for  $m^*$  correspond to those found in Fig. 5.3). In Fig. 5.9 one sees that the approximation yields satisfying results for a smaller choice of  $U$  (the maximum of the unapproximated values of  $m^*$  then is close to  $n = 0.5$ ).



**Figure 5.8:** Parameters:  $t_1 = 1$ ,  $t_1 = 0.8$ ,  $U = 1$



**Figure 5.9:** Parameters:  $t_1 = 1$ ,  $t_1 = 0.8$ ,  $U = 0.1$ . We could not calculate a meaningful numerically exact result for  $n = 0.9$ . Therefore it is missing in this plot.

## 6 Summary and concluding remarks

**Summary** We proved the existence of a new type of transition in the orbital order of a spin-polarized two-band Hubbard model evaluated with the Gutzwiller approximation, and showed that this effect occurs continuously for arbitrarily weak interactions. We calculated an approximate expression for the magnitude of the orbital polarization and gave its explicit dependence on  $t_1$  and  $t_2$ . Its dependence on  $U$  was calculated to be quadratic for small  $U$ . In the numerical part we confirmed these results. There it also became obvious that the magnitude of the orbital polarization is indeed small. The general approach to the problem with a Taylor expansion in  $m$  is therefore justified. Furthermore we showed that the effect is not present in the Hartree Fock approximation. In the Gutzwiller approximation there exist particular cases for which the effect is not going to occur. We explicitly listed those cases.

**Remark 1** In principle we can now use our results to calculate the magnitude of the orbital polarization for lattices with arbitrary dimensions and geometries by inserting the according DOS in our expressions. Also there is no reason why the adjustment of the model system (see chapter 2) should constitute a restriction to generality, since the effect occurs in an unadjusted system, too. The adjustment does not affect the determining equations except for a constant. However we state that – compared to the initial polarization of a system with  $t_1 \neq t_2$  – the transition we investigated is a small effect. If one wants to increase the magnitude of the effect one sees that this effort is – w.r.t. an adjustment of  $t_1$  and  $t_2$  – limited by  $\max_{t_1, t_2 \geq 0} \frac{t_1 - t_2}{t_1 + t_2} = \lim_{t_2 \rightarrow 0} \frac{t_1 - t_2}{t_1 + t_2} = 1$ , see (4.41). One will therefore not be able to construct a system which shows a strong orbital polarization by changing  $t_1$  and  $t_2$ . Perhaps this could be achieved with a special choice for the DOS, which remains to be investigated.

**Remark 2** We can *a posteriori* state that in our case the application of the GA is justified, as we can confirm the assumption that we deal with a weak-coupling phenomenon. In contrast to that, an investigation of the Stoner instability would not have produced realistic results as one would have to consider too high values of  $U$  for that the GA could be meaningfully applicable. Finally we state that it would also make sense to approach the model system in perturbation theory. The results of this alternative would be interesting to compare with our findings.

## *6 Summary and concluding remarks*



# Bibliography

- [1] A. Takahashi and H. Shiba, *J. Phys. Soc. Jpn.* **69**, 3328 (2000).
- [2] M. Greger, “Orbital order in a one-dimensional two-band Hubbard model”,  
F-Praktikum Teil B, Universität Augsburg, unpublished (2007).
- [3] P. F. J. Bünemann, K. Javorne-Radnoczi and F. Gebhard,  
*J. Phys.: Condens. Matter* **19**, 326217 (2007).
- [4] J. Hubbard, *Proc. R. Soc. London., Ser. A* **276**, 238 (1963).
- [5] J. Kanamori, *Prog. Theor. Phys.* **30**, 238 (1963).
- [6] M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963).
- [7] M. C. Gutzwiller, *Phys. Rev.* **137**, A1726 (1965).
- [8] D. Vollhardt, *Rev. Mod. Phys.* **56**, 99 (1984).
- [9] W. Metzner and D. Vollhardt, *Phys. Rev. B.* **37**, 7382 (1988).
- [10] W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).

## *Bibliography*

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