Rigorous Criteria for Ferromagnetism in Itinerant Electron Systems

Rainer Strack and Dieter Vollhardt
Institut für Theoretische Physik C, Technische Hochschule Aachen, D-52056 Aachen, Federal Republic of Germany
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We derive the first detailed, rigorous criteria for the stability of saturated ferromagnetism in the most general single-band model of itinerant electrons, valid for arbitrary translationally invariant lattices, at half filling. These conditions are given by inequalities for the model parameters. Of all interactions only the on-site and the exchange interaction are found to be essential. By the same approach we also derive rigorous criteria for the stability of saturated ferromagnetism in the Hubbard model with a magnetic field.

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Ferromagnetism is a quantum-mechanical many-body phenomenon caused by electronic interactions. Since the direct spin-spin interaction between electrons is very weak, ferromagnetism in itinerant electronic systems, e.g., in transition metals, must be due to a combination of the electrostatic Coulomb interaction and the Pauli principle. This was already known to Heisenberg in 1928 [1]. Nevertheless, until today it has not been possible to work out exact, detailed theoretical conditions for the occurrence of ferromagnetism in itinerant electronic systems. Such conditions must be derived from a microscopic band model of interacting electrons. To this end the simplest generic model of interacting electrons, the Hubbard model [2–4], where all interactions but the on-site term are neglected, was studied most intensively. However, even for this model secured knowledge about *ferromagnetic* phases exists only in special limits [5]. There do exist ferromagnetic solutions for the Hubbard model [6], based on various approximation schemes, but their stability is not proven. The importance of the neglected nearest-neighbor exchange interaction for the stabilization of ferromagnetism was stressed by Hirsch [7,8] and discussed by him and Campbell, Gammel, and Loh [9].

In this Letter we construct the first detailed, rigorous criteria for the stability of saturated ferromagnetism at $n=1$ valid for *arbitrary* translational invariant lattices with L sites and the *most general* single-band model of itinerant electrons with spin-independent interactions

$$\hat{H}=\sum_{i\neq j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+\tfrac{1}{2}\sum_{ijmn}\sum_{\sigma\sigma'} v_{ijmn}\hat{c}^{\dagger}_{i\sigma}\hat{c}^{\dagger}_{j\sigma'}\hat{c}_{n\sigma'}\hat{c}_{m\sigma}. \qquad (1)$$

The first term is a general kinetic energy due to hopping between two sites i,j, and the second term describes the electronic interaction, where matrix elements $v_{ijmn}=\langle ij|v_{ee}(\mathbf{r}-\mathbf{r}')|mn\rangle$ are expressed in terms of Wannier orbitals localized at sites i,j,m,n. As usual $\hat{c}^{\dagger}_{i\sigma}$ ($\hat{c}_{i\sigma}$) creates (annihilates) a σ electron at site i. We wish to know under which circumstances is the saturated ferromagnetic state $|\Psi_F\rangle=\prod_i\hat{c}^{\dagger}_{i\uparrow}|0\rangle$ the unique ground state of $\hat{H}$. The central question is then: For what choice of coupling parameters in (1) does $|\Psi_F\rangle$ become the lowest eigenstate? To find an answer we (i) transform (1) into a sum of positive-semidefinite operators, i.e., construct a lower bound E_l on the ground state energy (this is the hard part), (ii) show that $|\Psi_F\rangle$ is an eigenstate of (1), i.e., obtain an upper bound E_u, (iii) determine the conditions for $E_l=E_u$ [10], and (iv) prove the uniqueness of $|\Psi_F\rangle$.

We write (1) as $\hat{H}=\hat{H}^{1,2}+\hat{H}^{3,4}$ where $\hat{H}^{1,2}$ contains the sum over all 1- and 2-site terms and $\hat{H}^{3,4}$ involves all interactions involving 3 and 4 different sites. We first solve the problem for $\hat{H}^{1,2}$ and then include $\hat{H}^{3,4}$ afterwards. Because of translational invariance the (real) matrix elements in (1) depend only on the separation between sites, i.e., $t_{ij}\equiv t_{j-i}$, $v_{ijmn}\equiv v_{j-i,m-i,n-i}$. The 1- and 2-site contributions to the interaction are given by $U\equiv v_{iiii}$, $V_{j-i}\equiv v_{ijij}$, $X_{j-i}\equiv v_{iiij}$, $F_{j-i}\equiv v_{ijji}$, and $F'_{j-i}\equiv v_{iijj}$. Hence

$$\hat{H}^{1,2}=\sum_{i\neq j,\sigma} t_{j-i}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}+\tfrac{1}{2}\sum_{i\neq j}V_{j-i}\hat{n}_i\hat{n}_j+\tfrac{1}{2}\sum_{i\neq j,\sigma}X_{j-i}(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma})(\hat{n}_{i-\sigma}+\hat{n}_{j-\sigma})$$
$$+\tfrac{1}{2}\sum_{i\neq j,\sigma\sigma'}F_{j-i}\hat{c}^{\dagger}_{i\sigma}\hat{c}^{\dagger}_{j\sigma'}\hat{c}_{i\sigma'}\hat{c}_{j\sigma}+\tfrac{1}{2}\sum_{i\neq j,\sigma}F'_{j-i}\hat{c}^{\dagger}_{i\sigma}\hat{c}^{\dagger}_{i-\sigma}\hat{c}_{j-\sigma}\hat{c}_{j\sigma}, \qquad (2)$$

where $\hat{n}_{i\sigma}=\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ and $\hat{n}_i=\sum_\sigma\hat{n}_{i\sigma}$. While U parametrizes the on-site interaction and V describes the usual interaction between charges ($\equiv$ densities) at arbitrary sites $i\neq j$, the remaining interactions are off diagonal. Hence X_{j-i} corresponds to a density-dependent hopping between i and j, F_{j-i} is the familiar Heisenberg exchange integral [note that this interaction term may be written as $\sum_{i\neq j}F_{j-i}(-\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j-\frac{1}{4}\hat{n}_i\hat{n}_j)$, with spin operator $\hat{\mathbf{S}}_i$], and F'_{j-i} generates hopping of doubly occupied sites. Let us first discuss some special limits of (2), with $l=j-i$: *(1) On-site limit:* for $V_l=X_l=F_l=F'_l=0$ one recovers the Hubbard model with general hopping. *(2) Nearest-neighbor (NN) limit:* for $|l|=1$, with $t_1\equiv -t$, $V_1\equiv V$, $X_1\equiv X$, $F_1\equiv F$, and $F'_1\equiv F'$, Eq. (2) corresponds to a generalized Hubbard model where all NN interactions are included [7,9]. For $t=X=-V=-F=-F'=1$, $U\rightarrow U-Z$ one obtains the supersymmetric model of Essler, Korepin, and Schoutens [11].

We now rewrite (2), making repeated use of the opera-

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tor identity

$$\langle \hat{\Omega}^+\hat{\Lambda}+\hat{\Lambda}^+\hat{\Omega}\rangle = \langle(\alpha\hat{\Omega}^+ + \alpha^{-1}\hat{\Lambda}^+)(\alpha\hat{\Omega}+\alpha^{-1}\hat{\Lambda})\rangle - \alpha^2\langle\hat{\Omega}^+\hat{\Omega}\rangle - \alpha^{-2}\langle\hat{\Lambda}^+\hat{\Lambda}\rangle$$

for all $\alpha\neq 0$. Introducing the nonlocal operators

$$\hat{P}_{ij,\sigma} = (1-\hat{n}_{i-\sigma})\hat{c}_{i\sigma} + \lambda_1(1-\hat{n}_{j-\sigma})\hat{c}_{j\sigma}, \tag{3a}$$

$$\hat{Q}_{ij,\sigma} = \hat{n}_{i-\sigma}\hat{c}_{i\sigma} + \lambda_1 \hat{n}_{j-\sigma}\hat{c}_{j\sigma}, \tag{3b}$$

$$\hat{A}_{ij} = \alpha_{j-i}^{-1}(\hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}) + \lambda_2 \alpha_{j-i}(\hat{c}_{j\downarrow}\hat{c}_{i\uparrow} + \hat{c}_{i\downarrow}\hat{c}_{j\uparrow}), \tag{3c}$$

$$\hat{B}_{ij} = \hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \lambda_3 \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}, \tag{3d}$$

where

$$\lambda_1 = -\mathrm{sgn}(t_{j-i}),\quad \lambda_2 = \mathrm{sgn}(X_{j-i}+t_{j-i}),$$
$$\lambda_3 = \mathrm{sgn}(F'_{j-i} - \alpha_{j-i}^{-2}|X_{j-i}+t_{j-i}|),$$

and $\alpha_{j-i}\neq 0$ is real but otherwise arbitrary, it can be verified that

$$\hat{H}^{1,2} = \frac{1}{2}\sum_{i\neq j}\left[|t_{j-i}|\sum_{\sigma}(\hat{P}_{ij,\sigma}\hat{P}^{\dagger}_{ij,\sigma} + \hat{Q}^{\dagger}_{ij,\sigma}\hat{Q}_{ij,\sigma}) + |X_{j-i}+t_{j-i}|\hat{A}^{\dagger}_{ij}\hat{A}_{ij} + |\tilde{F}'_{j-i}|\hat{B}^{\dagger}_{ij}\hat{B}_{ij}\right] + \tilde{U}\hat{D} + \frac{1}{4}\sum_{i\neq j}|\tilde{V}_{j-i}|[\hat{n}_i + \mathrm{sgn}(\tilde{V}_{j-i})\hat{n}_j]^2 + \hat{C}_1 - \sum_{i\neq j}\tilde{F}_{j-i}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j. \tag{4}$$

Here $\hat{D}=\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the number operator for doubly occupied sites and $\hat{C}_1 = -\frac{1}{2}L\sum_{l\neq 0}[|\tilde{V}_l|\hat{n} + 4|t_l|(1-\hat{n})]$, with $\hat{n}=(1/L)\sum_{i\sigma}\hat{n}_{i\sigma}$. Furthermore,

$$\tilde{F}'_l = F'_l - |X_l+t_l|/\alpha_l^2,\quad \tilde{F}_l = F_l - \alpha_l^2|X_l+t_l|,$$
$$\tilde{V}_l = V_l - \frac{1}{2}(F_l + \alpha_l^2|X_l+t_l|)$$

for all $l\neq 0$, and

$$\tilde{U} = U - \sum_{l\neq 0}(4|t_l| + |\tilde{V}_l| + |X_l+t_l|/\alpha_l^2 + |\tilde{F}'_l|).$$

Except for the $\tilde{U}$ and $\tilde{F}$ terms and the unimportant $\hat{C}_1$, all terms in (4) are positive semidefinite. For $n=1$ it is seen that $|\Psi_F\rangle$ is an eigenstate of $\hat{H}^{1,2}$: (i) The P,Q,A,B terms have zero eigenvalue and hence $|\Psi_F\rangle$ even represents a ground state of these terms; (ii) from $\hat{D}|\Psi_F\rangle=0$ it follows that, for $\tilde{U}\geq 0$, $|\Psi_F\rangle$ is also a ground state of this term; (iii) the $\tilde{V}$ term has eigenvalues $L\sum_{l\neq 0}|\tilde{V}_l|$ for $\tilde{V}_l>0$ and zero for $\tilde{V}_l\leq 0$; since these values coincide with the lower bound of that term obtained by application of the Schwarz inequality $|\Psi_F\rangle$ is a ground state of the $\tilde{V}$ term too; (iv) $|\Psi_F\rangle$ is the unique ground state of the Heisenberg term provided $\tilde{F}_l>0$. For $\tilde{F}_l>0$ it is then clear that $|\Psi_F\rangle$ is the *unique* ground state of (4). That this is true even for $\tilde{F}_l=0$, provided $X_l\neq -t_l$ at least for $l=1$, can be proved by induction [12]. Hence for $n=1$, arbitrary $\alpha_l\neq 0$, and in the parameter regime,

$$F_1>0,\ \text{for}\ X_1=-t_1,\qquad F_l\geq \alpha_l^2|X_l+t_l|,\ \text{otherwise}, \tag{5a}$$

$$U\geq \sum_{l\neq 0}\left[4|t_l| + \left|V_l - \frac{F_l+\alpha_l^2|X_l+t_l|}{2}\right| + \frac{|X_l+t_l|}{\alpha_l^2} + \left|F'_l - \frac{|X_l+t_l|}{\alpha_l^2}\right|\right], \tag{5b}$$

the unique ground state of the Hamiltonian (4) is a fully polarized ferromagnetic state. The ground state energy is given by $E=\frac{1}{2}L\sum_{l\neq 0}(V_l-F_l)$. The above procedure can even be extended to include $\hat{H}^{3,4}$. In this case one has to introduce operators as in (3) that depend on 3 and 4 different site indices. Details will be presented elsewhere [13]. These contributions only *renormalize* the 2-site terms; i.e., they lead to the replacements $t_l\to t_l - \frac{1}{2}\sum_i' v_{il l}$, $V_l\to V_l + \frac{1}{2}W_l$ in (5a) and (5b), and $F_l\to F_l - W_l - 4\sum_i'|V_{l0i}|$ in (5a), where $W_l = \sum_i'(|v_{0li}| + |v_{lli}|) + \sum_{i,j}''|V_{ilj}|$ and the prime (double prime) on the sum implies $i\neq 0,l$ $(i\neq 0,l,j)$. This means that under the above conditions, given only by *inequalities*, the ground state of the general Hamiltonian (1) has saturated magnetization. This rigorous result holds for arbitrary translationally invariant lattices, i.e., even in $d=1$ [14]. Note that these are *sufficient* conditions; i.e., they do not rule out the stability of saturated ferromagnetism outside the above parameter range, e.g., in models where F is put to zero [5].

We now consider the NN limit, i.e., the Hubbard model with all NN interactions, with $\alpha_l=\alpha$, etc. The sum over l in (5b) then only leads to an overall factor Z, the number of NNs [15]. If (5a) is taken as an equality, α may be eliminated from (5); the parameter restriction for the stability of the saturated ferromagnet is then given by

$$\frac{U}{Z}\geq 4|t| + |V-F| + \frac{(X-t)^2}{F} + \left|F' - \frac{(X-t)^2}{F}\right|, \tag{6}$$

with $F>0$. For an fcc lattice this condition can be further improved [13]. We observe that of all interaction parameters *two* are most important for the stabilization of ferromagnetism: the on-site repulsion U and the exchange coupling F. This rigorous result supports the findings of Hirsch [7] which were obtained by mean-field calculations as well as numerical studies in $d=1$. For $V,X,F'=0$ Hirsch also derived an exact lower bound on F as a function of U below which the saturated ferromagnetic state on a d-dimensional hypercubic lattice is unstable [8]. Equation (6) shows that as long as F is nonzero (as in *real* physical systems), even if arbitrarily small, there exists a critical value of U above which the fully polarized state is stable. For a cubic lattice ($Z=6$) and the estimated values $V=2$ eV, $X=\frac{1}{2}$ eV, $F=F'=\frac{1}{40}$ eV [3] with 0.5 eV $\leq t\leq$ 1.5 eV one finds critical values between $U=24$ eV for $t=0.5$ eV and $U=528$ eV for $t=1.5$ eV. These values can be improved [13] by using new operators $\hat{P}_{ij,\sigma}=(1-\hat{n}_{n-\sigma})(\hat{c}_{i\sigma}+\lambda_1\hat{c}_{j\sigma})(1-\hat{n}_{j-\sigma})$ and $\hat{Q}_{ij,\sigma}=\hat{n}_{i-\sigma}(\hat{c}_{i\sigma}+\lambda_1\hat{c}_{j\sigma})\hat{n}_{j-\sigma}$ instead of (3a) and (3b). Thereby the critical U value for $t=0.5$ eV is lowered to $U=12$ eV, which is then actually in the range of physically relevant interaction parameters. A rigorous condition can even be derived for the stability of saturated ferromagnetism in the presence of a single hole ("Nagaoka state") [13]. This *itinerant* ferromagnetic state is found to be stable in a parameter regime very similar to (6), i.e., at *finite U*. Thereby Nagaoka's theorem for the Hubbard model [16] is generalized considerably. For $U\gg|t|,|V|,|X|,|F|,|F'|$ the condition (6) may be written as $\tilde{J}\equiv 4Z(X-t)^2/U-2F<0$. In this limit and for $\delta=1-n\ll 1$ the Hubbard model with all NN interactions can itself be transformed into an effective t-J model [13] by use of the usual transformation [17]. The effective Heisenberg coupling comes out as $J=4(X-t)^2/U-2F$ [18]. Since t and X can have quite similar values [19] the antiferromagnetic contribution to the effective coupling may, in principle, be very weak even if U is not extremely large. Hence, for $F>2(X-t)^2/U$ one obtains a *ferromagnetic t-J* model which is worth studying [20] for clear physical reasons. This model then allows one to treat also the more general cases $n<1$ and $T>0$, e.g., ferromagnetic states without full polarization. Apart from a factor Z the (nonrigorous) condition $J<0$, obtained from the t-J model, coincides with $\tilde{J}<0$; hence the rigorous condition is more restrictive.

Conditions (5) even hold for *complex* hopping matrix elements $t_l=|t_l|e^{i\phi_l}$. This case is relevant, for example, in the presence of magnetic flux. The two terms in the operators (3a)-(3c) then have to be multiplied by phase factors, e.g., $e^{\pm i\phi_l/2}$ in (3a) and (3b), which drop out in the end.

An external magnetic field B polarizes the electrons and will thus enhance any tendency towards ferromagnetism caused by the electronic interactions. In this case one should expect saturated ferromagnetism to become stable for finite U and arbitrary lattices even in the Hubbard model with NN hopping,

$$\hat{H}_{\rm Hub}=-t\sum_{\langle ij\rangle,\sigma}(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}+\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma})+U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}-B\sum_i(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}) \quad (7)$$

with $B>0$ along the z direction. Except for $d=1$ [21] nontrivial, rigorous criteria for the stability of a fully polarized ground state $|\Psi_F\rangle$ of (7) were so far not known. To derive such conditions for $n=1$ we rewrite the kinetic energy in (7) in terms of (3a) and (3b), with $\lambda_1=\mathrm{sgn}(\gamma t)$, and the new operators

$$\hat{R}_{ij,\sigma}=\hat{c}_{i\sigma}+\sigma\,\mathrm{sgn}[(1-\gamma)t]\hat{c}_{j\sigma},$$

$$\hat{O}_{ij,\sigma}=\alpha^{-1}\hat{c}_{i-\sigma}\hat{c}_{i\sigma}-\mathrm{sgn}(\gamma t)\alpha\hat{c}_{i-\sigma}\hat{c}_{j\sigma},$$

and

$$\hat{Y}=\sum_{\langle ij\rangle}[1-\tfrac{1}{2}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}+\hat{n}_{j\uparrow}-\hat{n}_{j\downarrow})]^2,$$

where $\alpha\neq 0$ and γ are real but otherwise arbitrary. The Hamiltonian (7) then takes the form

$$\hat{H}_{\rm Hub}=|t|\sum_{\langle ij\rangle}\left\{|1-\gamma|(\hat{R}_{ij,\uparrow}\hat{R}^\dagger_{ij,\uparrow}+\hat{R}^\dagger_{ij,\downarrow}\hat{R}_{ij,\downarrow})+|\gamma|\sum_\sigma(\hat{P}_{ij,\sigma}\hat{P}^\dagger_{ij,\sigma}+\hat{Q}^\dagger_{ij,\sigma}\hat{Q}_{ij,\sigma}+\hat{O}^\dagger_{ij,\sigma}\hat{O}_{ij,\sigma}+\hat{O}^\dagger_{ji,\sigma}\hat{O}_{ji,\sigma})\right\}+2\alpha^2|\gamma t|\hat{Y}$$
$$+\tfrac{1}{2}\alpha^2|\gamma t|\sum_{\langle ij\rangle}(\hat{n}_i-\hat{n}_j)^2+\tilde{U}\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}+\hat{C}_2-\tilde{B}\sum_i(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}), \quad (8)$$

where

$$\hat{C}_2=-ZL|\gamma t|[2(1-\hat{n})+\alpha^2(1+\hat{n})]-ZL|(1-\gamma)t|,$$

$$\tilde{U}=U-4Z|\gamma t|(1+1/2\alpha^2),$$

and

$$\tilde{B}=B-Z|(1-\gamma)t|-2Z\alpha^2|\gamma t|.$$

For $\tilde{U}\geq 0$ all but the last term and the unimportant $\hat{C}_2$ are positive semidefinite and have eigenvalue zero with respect to $|\Psi_F\rangle$. For $\tilde{B}>0$, $|\Psi_F\rangle$ is the unique ground state of the last term in (8), and for $\tilde{B}=0$ this can again be proved by induction in analogy to Ref. [10]. Hence it follows that for $\tilde{U},\tilde{B}\geq 0$, $|\Psi_F\rangle$ is the unique ground state of (7), with energy $E=-BL$. Eliminating α from the two inequalities and maximizing the ferromagnetic regime with respect to γ the fully polarized state at $n=1$ is seen to be stable for

$$\frac{U}{Z}\geq\begin{cases}4|t|(1+Z|t|/B), & 0\leq B\leq B^*,\\ 4|t|(3+\sqrt{8})(1-B/Z|t|), & B^*\leq B,\end{cases} \quad (9)$$

where $B^*=(\sqrt{2}-1)Z|t|$. Again the result holds for arbitrary translationally invariant lattices. The phase boundary is the convex envelope of the stability regimes obtained for $\gamma=0$ and $\gamma=1$, respectively. Note that for hypercubic lattices and $U=0$ the critical B value is $B=Z|t|$; i.e., (9) cannot be improved. The phase boundary of the fully polarized state is shown in Fig. 1 together with the result for $Z=2$ obtained from the Lieb-Wu equations [21]. The overall behavior, i.e., a linear and a $1/U$ dependence at small and large U, respectively, is the same. For $B\ll Z|t|$ the condition (9) is identical to (6) with $V=X=F'=0$ if F is replaced by $B/2Z$. Clearly, the exchange coupling F and the magnetic field B act in a very similar way. The conditions (9) even hold for $t=|t|e^{i\phi}$ as discussed above.

The same analysis can be applied to the spinless Falicov-Kimball model [22] at $n=1$. In this case the energy of the static electrons, E_f, corresponds to the magnetic field B in the Hubbard model, (7). Hence one can show [13] that for *any* $E_f\neq 0$ there exists a critical value

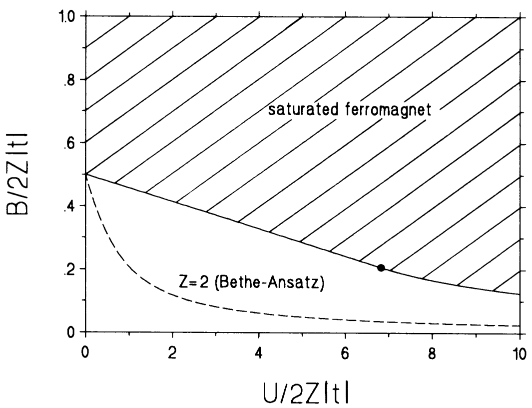

FIG. 1. Above the full line the ground state of the Hubbard model in a magnetic field B is proved to be fully polarized for arbitrary lattices with coordination number Z. Black dot: $B^* = (\sqrt{2}-1)Z|t|$; dashed line: boundary for $Z=2$ (Bethe-ansatz solution [21]).

of $U>0$ above which there are either only mobile or only static electrons, in close analogy to (9).

In summary, we derived explicit, sufficient conditions for the stability of a fully polarized ground state in the case of the most general one-band model of itinerant electrons with spin-independent interactions, as well as for the Hubbard in an external magnetic field. The results hold for arbitrary translationally invariant lattices and at half filling. We expect that our analysis can be carried through even in the case of band degeneracy which is generally expected to be essential for the stabilization of ferromagnetism in real physical systems. This would provide yet another step towards a genuine understanding of one of the most striking many-body phenomena in solid state physics.

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