Exact single spin flip for the Hubbard model in $d = \infty$

Götz S. Uhrig

Laboratoire de Physique des Solides, Université Paris-Sud, bât. 510, F-91405 Orsay

(March 23, 2022)

It is shown that the dynamics of a single $\downarrow$-electron interacting with a band of $\uparrow$-electrons can be calculated exactly in the limit of infinite dimension. The corresponding Green function is determined as a continued fraction. It is used to investigate the stability of saturated ferromagnetism and the nature of the ground state for two generic non-bipartite infinite dimensional lattices. Non Fermi liquid behavior is found. For certain dopings the $\downarrow$-electron is bound to the $\uparrow$-holes.

PACS: 75.10.Lp, 75.30.Kz, 71.30.+h, 71.27.+a

In the last years the limit of infinite dimensions $d \to \infty$, introduced by Metzner and Vollhardt for fermionic lattice models \cite{1}, has proved to be very useful in the investigation of strongly correlated electron systems \cite{2,3}. Its merit is an important simplification reducing lattice problems to effective one-site problems \cite{4} supplemented by a self-consistency condition \cite{5}. The limit $d \to \infty$ generates a mean-field theory which constitutes a very successful full approximation in $d < \infty$ \cite{1}. The mean-field keeps its frequency dependence (dynamic MFT) for local interactions \cite{1}. Thus important physics is retained. The effective one-site problem remains generally difficult to solve \cite{1}. So far, the metal-insulator transition \cite{6} and various ordering phenomena \cite{7,8,9,10,11} have been treated successfully. Recently, the investigation of polarized systems has been started \cite{12,13}.

Here the Green function of a $\downarrow$-electron interacting with the $\uparrow$-e$^-$ of filling $n$ (complete polarization) is calculated exactly. Two points will be addressed: (a) the stability of the Nagaoka state toward a spin flip; (b) the nature of the ground state.

(a): The understanding of ferromagnetism is an old problem at the origin of the Hubbard model \cite{2}. Saturated ferromagnetism (Nagaoka state) was proved for $U = \infty$ by Nagaoka for one e$^-$ above $n = 1$ \cite{14}. Ferromagnetism has been proved recently for a number of special cases: either the filling is such that the Fermi energy lies in a flat band \cite{15} or the situation corresponds to half-filling of one (sub)band \cite{16,17} or the limit $n \to 0$ for a Hubbard chain with two minima in the dispersion \cite{18} is considered. In $U$-$\delta$ diagrams (cf. fig. 1, 2), saturated ferromagnetism has been established by these results on vertical lines.

The range of stability of the Nagaoka state has been investigated extensively by variational methods see e.g. \cite{19,20}. More and more sophisticated trial wave functions for a flipped spin were used. Thereby, the region of possible local stability of the Nagaoka state was reduced considerably for various lattices. One has to rely so far on exact diagonalization data for small systems to estimate how far the variational phase boundaries are situated from the true ones; e.g. numerical results for the square lattice propose a doping above which the Nagaoka state is unstable at $U = \infty$ of $\delta_c = 0.195$ \cite{20} or $\delta_c = 0.22$ \cite{21} and the best rigorous upper bound is $\delta_c = 0.251$ \cite{22} at present.

The present work establishes exactly (in)stability of saturated ferromagnetism toward single spin flip for lattices in $d = \infty$ for all values of $\delta$. This allows to evaluate the quality of the variational approaches for these lattices.

(b): For certain values of $\delta$ the $\downarrow$-e$^-$ forms bound states with the $\uparrow$-holes which implies a non-Fermi liquid behavior. The mobility of the $\downarrow$-e$^-$ is reduced decisively: it does no longer diverge as it does in a Fermi liquid. The picture of bound particle-hole pairs is a possible interpretation of the metal-insulator transition occurring at $n = 1 \frac{1}{2}$.

Consider the local Green function for one $\downarrow$-e$^-$ $G(\omega) := G_{i,i;\downarrow}(\omega)$: $G_{i,i;\downarrow}$ is the Fourier transform of $-i(\hat{a}_{i;\downarrow}(t),\hat{a}_{i;\downarrow}(0))\Theta(t)$ ($\hbar$ is set to 1; $i$ can be any site).

This $\downarrow$-e$^-$ interacts in a Hubbard model with the Fermi sea of $\uparrow$-e$^-$. The expectation value is taken for the Fermi sea of $\uparrow$-e$^-$. Introducing the Liouville operator $L := [H, \cdot]$ \cite{23} $G(\omega)$ can be expressed as $G(\omega) = \langle \hat{a}_{i;\downarrow}(\omega - L)^{-1}\hat{a}_{i;\downarrow} \rangle$. The Morizwanzig projection method provides $G(\omega)$ as continued fraction (CF) with the static correlations of the Fermi sea as coefficients \cite{30}. So, $G(\omega)$ is in principle known. Yet, due to the rapidly increasing complexity of the coefficients with increasing order the CF is not tractable in $d < \infty$.

For $d \to \infty$, however, the self-energy is local \cite{2}. It is sufficient to consider $\Sigma(\omega) := \Sigma_{i,i;\downarrow}(\omega)$. The skeleton diagrams of $\Sigma(\omega)$ comprise only the local vertex $i \frac{1}{2}$ which interact only at the first site \cite{23} if their full local propagators are the same. This is the consistency condition: the chain Green function of the first site $G_{\lambda}(\omega)$ and the local lattice Green function are equal: $G_{i,i;\downarrow}(\omega) = G_{\lambda}(\omega), \lambda \in \{\uparrow, \downarrow\}$ \cite{23}. The matrix elements of the chain have to be determined such that the consistency is fulfilled. So, we are facing two nested problems: solving the consistency condition to find the matrix elements of the chain, and solving the one-site problem to find the self-energy.

For a single $\frac{1}{2} \downarrow$-e$^-$ the two problems can be solved by iterating a straightforward procedure. First, we state that the matrix elements of the chain describing the $\uparrow$-e$^-$ are those of the non-interacting problem since the $\uparrow$-e$^-$ do not interact with themselves (Recall that the ground state considered is the Fermi sea of $\uparrow$-e$^-$). So these ma-
trix elements, i.e. local energies and nearest neighbor hopping elements, are those of the CF \((a_i, b_i) \) of the non-interacting lattice DOS \(\rho(\omega)\) as weight function \(\sum\), i.e. the CF of \(G^0(\omega)\), the non-interacting local propagator.

Second, we know from Dyson’s equation that
\[
G(\omega) = G^0(\omega - \Sigma(\omega)) \quad \text{for the lattice, and} \quad g(\omega) = \frac{g^0(\omega)}{1 - g^0 \Sigma(\omega)} \quad \text{for the chain (\downarrow spin index omitted).}
\]
The identity of the local lattice proper self-energy and of the equivalent lattice proper quantity is obtained. Hence the consistency condition requires
\[
G^0(\omega - \Sigma(\omega)) = \frac{g^0(\omega)}{1 - g^0 \Sigma(\omega)}.
\]
Knowing the first CF coefficient pair \((a_0, b_0)\) of \(G^0(\omega)\), i.e. \(G^0(\omega) = (\omega - a_0 - b_0^2 g^0(\omega))^{-1}\), the consistency is equivalent to \(g^0(\omega) = (\omega - a_0 - b_0^2 g^0(\omega))^{-1}\) and
\[
g^0(\omega) = G^0(\omega - \Sigma(\omega)).
\]
By\(\mathbf{[1]}\) further CF coefficients \((x_i, y_i), i > 0,\) of \(g^0\) can be calculated from the CF coefficients \((s_i, t_i)\) of \(\Sigma\) by tridiagonalization. Note to this end that \(\mathbf{[4]}\) can be viewed as the Green function belonging to the one-particle Hamiltonian of a semi-infinite chain (CF of \(G^0\)) with the replicas of the chain of the CF of \(\Sigma\) attached to each site. The crucial point is that \((s_0, t_0)\ldots(s_n, t_n)\) are sufficient to calculate \((x_0, y_0)\ldots(x_{n+1}, y_{n+1})\).

Third, for the calculation of \(\Sigma(\omega)\) the projection method \(\mathbf{[3]}\) provides
\[
\Sigma(\omega) = U + U^2 \langle \hat{\Sigma}_{0\uparrow} Q(\omega - QLQ)^{-1} Q \hat{\Sigma}_{0\uparrow} \rangle 0 \quad (2)
\]
where \(\downarrow \) stands for the Fermi sea of \(\uparrow\)-e\(^{-}\) plus the \(\downarrow\)-e\(^{-}\) at the first site of the chain; \(\hat{\Sigma}_{0\uparrow} := \hat{c}_{0\uparrow} \hat{c}_{0\uparrow}^\dagger; Q\) projects out states without any particle-hole excitation, \(U\) is the interaction, and \(L\) is the commutation with
\[
\hat{H}_{\text{chain}} = U \hat{\Sigma}_{0\uparrow} \hat{\Sigma}_{0\downarrow} + \sum_{i=0}^{\infty} a_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} + b_i (\hat{c}_{i+1\uparrow}^\dagger \hat{c}_{i\uparrow}^\dagger + \text{h.c.})
\]
\[
+ \sum_{i=0}^{\infty} x_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} + y_i (\hat{c}_{i+1\uparrow}^\dagger \hat{c}_{i\downarrow} + \text{h.c.}).
\]

The essential difference to the problem at finite density of \(\downarrow\)-e\(^{-}\) is that for a single \(\downarrow\)-e\(^{-}\) the ground state \(\downarrow\) is known beforehand. The CF of \(\mathbf{[3]}\) is found again by tridiagonalization, i.e., the Lanczos algorithm is used with \(Q \hat{\Sigma}_{0\uparrow} \rangle 0\) as first state. The subspaces reached by the iterative application of \(QLQ\) are spanned by states which are products of equal numbers of \(\uparrow\)-creation and \(\uparrow\)-annihilation operators plus one \(\downarrow\)-creation operator on certain chain sites acting on the \(\uparrow\)-Fermi sea. Components without any particle-hole excitation are projected out. The crucial point is that \((x_0, y_0)\ldots(x_{n+1}, y_{n+1})\) are sufficient to calculate \((s_0, t_0)\ldots(s_{n+1}, t_{n+1}).\)

Hence, the nested problems of the consistency and of the effective one-site problem can be solved by alternating tridiagonalization steps for \(\mathbf{[1]}\) with steps for \(\mathbf{[4]}\).

Results will be presented for generalizations of the \(d = 3\) fcc lattice. One is interested in non-bipartite, electron doped lattices for their enhanced tendency toward ferromagnetism due to their asymmetric DOS with finite lower band edge \(\mathbf{[25, 26]}\). In contrast, the Nagaoka state is even completely unstable for the hypercubic lattice in \(d = \infty \mathbf{[24]}\). The properties of the lattice are essential for ferromagnetism. Finding stable ferromagnetism on non-bipartite lattices with local \(\Sigma\) is thus no contradiction to the robustness of local Fermi liquids \(\mathbf{[22]}\) in the \(d = 3\) continuum limit (spherical Fermi surface corresponding to \(n \rightarrow 0\) on the sc lattice). Additionally, Fermi liquid (FL) theory is not valid for all \(\delta\) and \(U\), see below and ref. \(\mathbf{[14]}\).

For simplicity, we consider
\[
\hat{H}_{\text{kin}} = t \sum_{(i,j), \lambda} \hat{a}_{i\lambda}^\dagger \hat{a}_{j\lambda}^\dagger, \quad \langle i, j \rangle \text{nearest neighbors with } t > 0 \quad \text{and} \quad n < 1 \text{ which is equivalent to } n > 1 \text{ and the usual } t < 0. \quad \text{A large DOS at the lower band edge is favorable for the Nagaoka state since it lowers the kinetic energy necessary for polarization.}
\]

The half hypercubic (hh) lattice is made of the even sites of the hypercubic (hc) lattice. Nearest-neighbor sites are linked by \(t\), sites at distance 2 are linked by \(t/2\). Then the dispersions are related by \(\varepsilon_{\text{hh}}(k) = \varepsilon_{\text{hc}}^2(k) - 1\) if \(t = 1/d\) on the hh and \(t = 1/\sqrt{2d}\) on the hc. Hence
\[
\rho_{\text{hh}}(\omega) = \rho_{\text{hc}}(\sqrt{1 + \omega})/\sqrt{1 + \omega} \mathbf{[33]} \quad \text{(recall } \rho_{\text{hc}}(\omega) = \exp(-\omega^2/2)/\sqrt{2\pi} \text{ for } d \rightarrow \infty \mathbf{[1]}).\]

Omitting the \(t/2\) hops leaves the DOS for \(d = \infty\) essentially unchanged. Yet the dispersion acquires a term \(-t \sum_{i=1}^{d} \cos(2k_i)\) which leads to a foot extending down to \(\omega = -2\). On \(d \rightarrow \infty\) the weight of this foot vanishes \(\mathbf{[33]}\), yet the foot is decisive for the single spin flip energy for any \(d < \infty\). The hh with foot in \(d = 3\) is the fcc lattice and in \(d = 2\) a square lattice.

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**FIG. 1.** Half hypercubic lattice: above the solid line the Nagaoka is stable toward spin flip. Main figure: hh without foot; dashed-dotted: variational result from \(\mathbf{[1]}\). Inset: hh with foot; maximum doping \(\delta_c = 0.4330\); minimum interaction \(U_{\text{red}} = 0.5809\); \(U_{\text{red}} := U/(U + U_{\text{BR}})\) with \(U_{\text{BR}} = 6.8588\).

The sites of a new layer of the laminated (lam) lattice are above the interstices of the layer below. The basis vectors are defined by \(b_{n+1} = (n + 1)^{-1} \sum_{i=1}^{n} b_i + \sqrt{(2 + n)/(2 + 2n)} e_{n+1}\) with \(b_1 = e_1\), where \(e_i\) are cubic unit vectors \(\mathbf{[34]}\). On scaling \(t = 1/d\), one yields for \(d \rightarrow \infty\) the exponential DOS \(\rho_{\text{lam}}(\omega) = \exp(-\omega^2/2 + \delta)^{-1}\)
1)Θ(ω + 2)/2. The lam in d = 3 is the fcc lattice, in
d = 2 it is the triangular lattice. Hence it is even a
better generalization of the known non-bipartite lattices
than the hh.

In figs. 1, 2 the exact phase boundaries above which the
Nagaoka state is locally stable are shown. To compare
different lattices the reduced interaction
\( U_{\text{red}} := U/(U + U_{\text{BR}}) \) is used where
\( U_{\text{BR}} \) is defined from the kinetic energy
at half-filling: \( U_{\text{BR}} := -16 \int_{-\infty}^{\infty} \omega \rho(\omega) d\omega \). The result
(inset fig. 1) agrees with the \( T \to 0 \) extrapolation to
saturated magnetization of QMC data for the hh lattice
at \( \delta = 0.42, U_{\text{red}} = 0.45198 \). [14]

The transition interaction is found from the zero of the
spin flip energy \( E_{\text{SF}} = \omega_0 - \mu \). Taking out a \( \uparrow \)-
electron gains \( \mu \) and inserting a \( \downarrow \)-electron costs at least \( \omega_0 \) where
\( \omega_0 \) is the lower band edge of \( G(\omega) \). The band edge \( \omega_0 \) is
computed by extrapolating the approximate band edge
\( \omega_a(j) \) (j depth of the CF, here \( j \leq 53 \)) to \( j = \infty \). The
approximate values are found from
\[
\varepsilon_b = \omega_a(j) - \Sigma_n(\omega_n; j).
\]
They always lie below the band edge \( \omega_S(j) \) of \( \Sigma_n(\omega; j) \):
\( \text{Re} \Sigma_n(\omega; j) \) diverges to \( -\infty \) on \( \omega \to \omega_S(j) \) because the
spectral density of \( \Sigma_n(\omega; j) \) consists of \( \delta \)-peaks for \( j < \infty \).
Thus [1] has a zero in the interval \( (-\infty, \omega_S(j)) \) even
though the weight of lowest lying \( \delta \)-peak may become
arbitrarily small on \( j \to \infty \). For \( j = \infty \), however, \( \varepsilon_b > \omega_0 - \Sigma_0(\omega_0) \)
is possible since the spectral density of \( \Sigma \) is generally continuous. The inequality implies that
\( G_0(\omega - \Sigma) \) acquires an imaginary part due to the imaginary part of \( \Sigma \) and not because the lowest scattering state, renormalized by \( \Sigma \), can be excited. The latter,
however, is a necessary condition for quasi-particles to
be the elementary excitations and thus for the applicability of FL theory.

The non-solid lines are variational results. The dashed
curves result from a scattering type ansatz
\[
\psi(q) = \sum_{j,i} e^{-iqr_j} \left( \frac{u_i}{N} \hat{a}^\dagger_{j,i} + \hat{a}_{j+1,i+j} \hat{a}^\dagger_{j,i+j} \right) |\text{FS}'\rangle
\]
where \( |\text{FS}'\rangle = \hat{a}^\dagger_{kF,i}|\text{FS}\rangle \) \( (k_F \) Fermi wave vector, \( N \) #
of sites) [35]. The variational variables are \( u_1 \).
The optimum is attained for a \( q \) with \( \varepsilon(q) = \varepsilon_b \). The
dashed-dotted lines come from an ansatz for a bound state between a \( \downarrow \)-electron and a \( \uparrow \)-hole
\[
\Phi(q) = \sum_{k \in \text{FS}} v_k \hat{a}^\dagger_{k+q,i} \hat{a}^\dagger_{k,i} |\text{FS}\rangle.
\]
The variational variables are \( \{v_k\} \). The optimum is found
for \( q \to 0 \) unlike the results for the square lattice [24]
where \( q = (0, \pi) \) was optimal.

Comparison of the solid lines with the dashed ones in
figs. 1, 2 reveals that an ansatz like [11] gives a good idea
what the stability region looks like for different lattices.
One recognizes the influence of the singularity of \( \rho(\omega) \) at
\( \varepsilon_b \): an inverse square root leads to a Nagaoka state even
for \( n \to 0 \) and \( U \to 0 \), a constant implies a Nagaoka state
for \( n \to 0 \) but only for \( U \to \infty \) (in the exact result), and
a foot, i.e. a low DOS at \( \varepsilon_b \), leads to \( \delta_c < 1 \). The ansatz
[6] fails especially to describe the behavior at large \( U \).

Close to \( \delta = 0 \), the dashed-dotted lines of [1] obviously
capture the right physics since they are asymptotic to the
exact curves. This leads to the hypothesis that the \( \downarrow \)-electron
is actually bound to the \( \uparrow \)-holes. It is supported by the
fact that for small \( \delta \) the curves for the hh with and without
foot are numerically indistinguishable. The energy of a bound state is not changed by a foot of infinitesimal weight whereas the energy of the lowest scattering state is.

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foot are numerically indistinguishable. The energy of a bound state is not changed by a foot of infinitesimal weight whereas the energy of the lowest scattering state is.
since $\varepsilon_b > \omega_0 - \Sigma(\omega_0)$. The physical interpretation suggested from the success of the bound state ansatz (1) for small $\delta$ and large $U$ is that bound $\downarrow-e^-\uparrow$-hole states replace the quasiparticles as elementary excitations. From $1 = \varepsilon_b - \omega_0 + \Sigma(\omega_0)$ (cf. fig. 3) we find the doping $\delta = 0.044$ below which the exact curves for the hh with and without foot coincide in fig. 1.

The interpretation of $\varepsilon_b > \omega_0 + \Sigma(\omega_0)$ as indication for a binding phenomenon is corroborated by the resulting finite conductivity/mobility $\sigma$ of the $\downarrow-e^-$. For $T \rightarrow 0$, one has $\sigma \propto \text{Im} G(\omega_0)/\text{Im} \Sigma(\omega_0)$ [36]. This is bounded from above according to $\text{Im} G(\omega_0)/\text{Im} \Sigma(\omega_0) = \int_{\omega_0}^{\infty} \rho_0(\omega)(\omega - \omega_0 + \Sigma(\omega_0))^{-2} d\omega < (\varepsilon_b - \omega_0 + \Sigma(\omega_0))^{-2}$. If the system displayed no binding phenomenon (e.g. in a FL) one would have a diverging $\sigma$ since $\text{Im} \Sigma(\omega)$ vanishes generally faster than $\text{Im} G(\omega)$ on $\omega \rightarrow \omega_0$.

In summary, this work introduced a method (nested application of two tridiagonalisations) to calculate the dynamics of a single spin flip as continued fraction for $d \rightarrow \infty$ or, equivalently, for the local approximation. The usual, cumbersome self-consistency condition is solved in this case exactly.

By this method, the region of local stability of saturated ferromagnetism was computed exactly for two nonbipartite lattices and compared to variational results. The latter yield a good qualitative impression of the local stability region but fail to describe it quantitatively.

For small $\delta$ (large $U$) a binding phenomenon which is incompatible with Fermi liquid behavior was found. In this regime, the mobility of the $\downarrow-e^-$ remains finite. This non Fermi liquid behavior certainly deserves further investigation.

The author acknowledges stimulating discussions with E. Müller-Hartmann, Th. Hanisch, B. Kleine, and P. Wurth as well as with H. J. Schulz and A. Mielke. It was supported by the SFB 341 of the DFG and by the EEC, grant ERBCHRXCT 940438.

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