Magnetic Properties of the $t$-$J$ Model in the Dynamical Mean-Field Theory

Th. Pruschke, Q. Qin, Th. Obermeier and J. Keller

Institut für Theoretische Physik, Universität Regensburg,
D-93040 Regensburg, Germany

January 13, 2022

Abstract

We present a theory for the spin correlation function of the $t$-$J$ model in the framework of the dynamical mean-field theory. Using this mapping between the lattice and a local model we are able to obtain an intuitive expression for the non-local spin susceptibility, with the corresponding local correlation function as input. The latter is calculated by means of local Goldstone diagrams following closely the procedures developed and successfully applied for the (single impurity) Anderson model. We present a systematic study of the magnetic susceptibility and compare our results with those of a Hubbard model at large $U$. Similarities
and differences are pointed out and the magnetic phase diagram of the $t$-$J$ model is discussed.

Pacs numbers: 71.27+a, 71.28+d, 75.10.LP
1 Introduction and survey.

The description of strongly correlated electron systems involves by and large three different classes of models. First one may consider a system consisting of uncorrelated delocalized electronic states hybridizing with localized states subject to a strong Coulomb repulsion. This situation is modeled by the well known periodic Anderson model [1] frequently used to describe the so-called heavy-fermion compounds [2]. The second important situation occurs when the delocalized states themselves feel locally such a strong repulsion. In that case one is led to the single-band Hubbard model [3], originally set up to describe (ferro-) magnetism and metal-insulator transitions in 3d transition-metals compounds like V$_2$O$_3$ but recently also used for the high-T$_c$ superconductors. Another interesting kind of system is obtained if in addition to those local correlations a nonlocal magnetic exchange is included. This is the domain of the so-called $t$-$J$ model [4] which is frequently taken as an alternative to the Hubbard model to describe the properties of the cuprate superconductors. It is this model we want to study more closely in this paper. Although the $t$-$J$ model may be viewed as an effective Hamiltonian for the low-energy properties of the Hubbard model in the limit of large local Coulomb energy [5], i.e. vanishing effective magnetic exchange, both models are expected to differ fundamentally for increasing exchange interaction.

The Hamiltonian of the $t$-$J$ model reads

$$ H_{t-J} = -\frac{t^*}{\sqrt{2Z}} \sum_{\langle ij \rangle_\sigma} X_{1,0}^{(i)} X_{0,1}^{(j)} + \frac{J^*}{Z} \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j. $$

In equation (1), $X_{M,M'}^{(j)} = |j, M\rangle \langle j, M'|$ are the standard Hubbard operators [3] acting
on states with quantum number $M \in \{0, 1\sigma\}$ on site $j$, i.e. double occupancy of a site is strictly forbidden, and $\vec{S}_i$ denotes the spin operator on site $i$. The sums in the Hamiltonian (1) are on nearest neighbors only. The transfer and exchange integrals $t$ and $J$ have been rescaled with the coordination number $Z$ of the system to guarantee a physical meaningful result for large spatial dimensions to be introduced later. Note that for $J^* = 0$ the model (1) is the Hubbard model in the limit $U = \infty$. An additional density-density interaction frequently included in the model (1) has been dropped here for reasons of convenience.

Although the model (1) looks rather simple, relatively little is known exactly about its properties. In contrast to the Hubbard model, it is not even exactly solvable in $d = 1$ except for the two special points $J^* = 0$ (Hubbard model) and $J^* = 2t^*$ (supersymmetric $t$-$J$ model). Nevertheless, exact diagonalization studies showed that the $t$-$J$ model for $d = 1$ and $T = 0$ is a Luttinger liquid for all $J < J_{PS}$, while for $J > J_{PS}$ one finds phase separation into an electron and hole rich region. Interestingly, close to this boundary, the ground state of the $t$-$J$ model is dominated by superconducting pair correlations, while for smaller $J$ antiferromagnetic correlations are strongest.

Obviously, this would make the $t$-$J$ model an interesting candidate for explaining e.g. high-temperature superconductivity. Unfortunately, the results for $d = 1$ suggest a much too large value of $J^*/t^* \sim 3 \ldots 4$ for this scenario. The interesting question thus is how these features survive in $d > 1$ and especially to what extent phase separation might occur at much lower values of $J$, as suggested by e.g. high-temperature expansions.
While in $d = 1$ the combination of exact diagonalization and tools of conformal field theory provides a powerful framework to extract informations about the asymptotics of the macroscopic system, similar methods do not exist in $d > 1$. Quantum Monte Carlo techniques, too, cannot be applied for realistic lattice-sizes and temperatures due to a severe minus-sign problem. Thus most informations about the properties of the $t$-$J$ model come from high-temperature expansions, which are restricted to relatively large values of $J^*$ and $T$ [11,12], and exact diagonalization studies for small two-dimensional systems [12,13]. The finite system size in the latter method possibly prevents one from resolving dynamically generated low-energy features, which one may especially expect close to half filling [14,15,16]. Moreover, to interpret results for dynamic quantities calculated with this method one generally needs additional information from other techniques about the general structures to be expected. Clearly, a different approach to obtain results in the thermodynamic limit is needed.

Usually, a mean-field theory provides a reliable tool to study at least the qualitative features of models in theoretical solid-state physics. However, until recently a thermodynamically consistent mean-field theory like for spin systems did not exist for fermionic models like the $t$-$J$ model [1]: While the magnetic exchange term could in principle be handled by the standard Hartree factorization it is a priori not obvious how to treat the correlated hopping introduced by the first term in the model [1] consistently within this ansatz. Different schemes, usually involving slave-boson techniques, have been proposed [12]. These methods treat the local dynamics induced by the correlations rather poorly and a systematic inclusion of fluctuations around the static limit
to incorporate lifetime effects is very cumbersome and has not been successful yet \[17\].

Over the past three years, however, a novel scheme was introduced to define a thermodynamically consistent mean-field theory for correlated systems that preserves the local dynamics exactly \[20,21,22\]. In this contribution we shall use this so-called “dynamical mean-field theory” to study the mean-field magnetic properties of the \(t-J\) model (1). The paper is organized as follows. In the next section we will briefly introduce the dynamical mean-field theory and derive expressions for the magnetic susceptibility of the \(t-J\) model. We then present results on the magnetic properties and compare them to the large-\(U\) Hubbard model. A summary and discussion concludes the paper.

## 2 Theoretical background

Since the pioneering work of Metzner and Vollhardt \[18\] and subsequently Müller-Hartmann \[19\], Brandt and Mielsch \[20\] and Janiš \[21\] it is known that a correlated lattice model can be mapped onto an effective impurity system in the limit \(d \to \infty\). This is one consequence of the important aspect of this limit, namely that the irreducible one-particle self energy is purely local \[18,19\] and a functional of the local propagator only \[20,21,22,23\]. This property can be used to rewrite the lattice problem in such a way that one is left with the solution of an effective single-impurity Anderson model (SIAM), where the free bandstates are replaced by an effective medium obtained from the full problem with the site under consideration removed \[20,21,22,23\]. The one-
particle Greens function or equivalently the one-particle self energy of the system are then given by the corresponding quantities of the effective single-site problem. We shall see later, that one can also calculate the two-particle correlation functions of the lattice system with the help of those of the effective SIAM. Note that this effective theory preserves the dynamics introduced by the local correlations and thus is still highly nontrivial since there does not exist a complete solution for the SIAM. However, there exist at least different numerical exact techniques like quantum Monte Carlo and controlled perturbational approximations to solve this local model \[14,24\]. All these methods can then in turn be used to provide a solution of correlated lattice models in the thermodynamical limit. This approach has become known as the dynamical mean-field theory. The name is based on the observations that (i) the limit \(d = \infty\) provides a canonical starting point for the construction of a thermodynamically consistent mean-field theory \[25\] and (ii) in contrast to a standard mean-field theory (like e.g. the one for the Heisenberg model) one obtains a complex, frequency dependent function as molecular field due to the dynamical nature of the local Coulomb repulsion. Note that with the same arguments one also finds that the contribution to the one-particle self-energy due to interactions like the spin exchange in the model \(1\) is given by the corresponding Hartree diagram only and thus is also purely local and in addition static \[19\]. The latter statement means that for \(d = \infty\) the \(t\)-\(J\) model in the paramagnetic phase (i.e. when \(\langle S^z_i \rangle = 0\)) is identical to the Hubbard model with \(U = \infty\). Regarding the one-particle properties in this regime we thus expect the well known features of the Hubbard model \[14\]. The situation of course changes as soon as one has a transition
into a magnetic state which will be discussed elsewhere \[13\].

### 2.1 Susceptibility for the $t$-$J$ model

For our purposes it is convenient to represent the transverse spin susceptibility of the $t$-$J$ model as

$$\chi^J_{\bar{q}}(i\nu_n) = \frac{1}{\beta^2} \sum_{\omega_n, \omega_m} \chi_{\bar{q}}(i\omega_n, i\omega_m; i\nu_n) e^{i(\omega_n + \omega_m) n^\dagger} ,$$  \hfill (2)

where $\chi_{\bar{q}}(i\omega_n, i\omega_m; i\nu_n)$ is the spatial Fourier transform of the particle-hole propagator

$$\chi_{ij}(i\omega_n, i\omega_m; i\nu_l) = \frac{1}{\beta} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 e^{-i\omega_m(\tau_1 - \tau_2)} e^{-i\omega_n(\tau_3 - \tau_4)} e^{-i\nu_l(\tau_2 - \tau_4)}$$

$$\langle T_{\tau_1} c_{i\uparrow}^{\dagger}(\tau_4) c_{i\downarrow}(\tau_3) c_{j\downarrow}(\tau_2) c_{j\uparrow}(\tau_1) \rangle_{tJ} .$$  \hfill (3)

In equations (2) and (3) $i\omega_n$ and $i\omega_m$ denote Fermi Matsubara frequencies and $i\nu_n$ a Bose Matsubara frequency. Quite generally, by introducing the irreducible two-particle self energy $\Gamma^{\uparrow\downarrow}_{ij}(i\omega_n, i\omega_m; i\nu_l)$, the particle-hole propagator (3) can formally be written as

$$\chi_{ij}(i\omega_n, i\omega_m; i\nu_l) = \beta \chi^{(0)}_{ij}(i\omega_n; i\nu_l) \delta_{n,m}$$

$$+ \frac{1}{\beta} \sum_{lk, i\omega_p} \chi^{(0)}_{ll}(i\omega_n; i\nu_l) \Gamma^{\uparrow\downarrow}_{lk}(i\omega_n, i\omega_p; i\nu_l) \chi_{kl}(i\omega_p, i\omega_m; i\nu_l) .$$  \hfill (4)

Here, $\chi^{(0)}_{ij}(i\omega_n; i\nu_n) = -G_{ij}(i\omega_n) G_{ji}(i\omega_n + i\nu_n)$ represents the unperturbed part of the particle-hole propagator and $G_{ij}(i\omega_n)$ the full one-particle Greens function of the system.

Using standard techniques of field theory [20], one can express the irreducible
particle-hole self energy as functional derivative of the one-particle self energy with respect to the one-particle propagator. In combination with the observation, that within the dynamical mean-field theory (DMFT) (i) the one-particle self energy is purely local and (ii) the exchange term \( J^* \) enters the one-particle self energy only on the Hartree level it follows that the two-particle self energy acquires the particularly simple form

\[
\Gamma_{lk}^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_l) = -\frac{J^*}{Z} \delta_{|i-j|,n,N} + \Gamma_{lk}^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_l) .
\]  

(5)

The non-trivial second term is the irreducible particle-hole self energy for \( J^* = 0 \), i.e. for the \( U = \infty \)-Hubbard model. Note that within the DMFT this quantity is also purely local \[20]\!

Inserting the result (5) into the expression (4) and transforming into \( \vec{q} \)-space, we obtain as transverse magnetic susceptibility of the \( t-J \) model in the DMFT

\[
\chi_{\vec{q}}(i\omega_n, i\omega_m; i\nu_n) = \beta \chi_{\vec{q}}^{(0)}(i\omega_n; i\nu_n) \delta_{nm} + J_{\vec{q}} \chi_{\vec{q}}^{(0)}(i\omega_n; i\nu_n) \frac{1}{\beta} \sum_p \chi_{\vec{q}}(i\omega_p, i\omega_m; i\nu_n) \\
+ \frac{1}{\beta} \sum_p \chi_{\vec{q}}^{(0)}(i\omega_n; i\nu_n) \Gamma_{\vec{q}}^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_n) \chi_{\vec{q}}(i\omega_p, i\omega_m; i\nu_n) .
\]

(6)

In equation (6) \( J_{\vec{q}} \) denotes the Fourier transform of \( -\frac{J^*}{Z} \delta_{|i-j|,n,N} \). For the case of a simple hyper-cubic lattice one e.g. obtains \( J_{\vec{q}} = -\frac{J^*}{d} \sum_{l=1}^{d} \cos(q_l \cdot a) \).

The susceptibility (6) contains as one contribution the susceptibility of the Hubbard
model in the limit $U = \infty$ given by [22]

$$\chi_q^{HM}(i\omega_n, i\omega_m; i\nu_n) = \beta\chi_q^{(0)}(i\omega_n; i\nu_n)\delta_{nm}$$

$$+ \frac{1}{\beta} \sum_p \chi_q^{(0)}(i\omega_n; i\nu_n)\Gamma^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_n)\chi_q^{HM}(i\omega_p, i\omega_m; i\nu_n).$$

(7)

It is now straightforward to show that with the help of expression (7) equation (6) can be rewritten as

$$\chi_q(i\omega_n, i\omega_m; i\nu_n) = \chi_q^{HM}(i\omega_n, i\omega_m; i\nu_n)$$

$$+ J_q\frac{1}{\beta} \sum_l \chi_q^{HM}(i\omega_n, i\omega_l; i\nu_n)\frac{1}{\beta} \sum_p \chi_q(i\omega_p, i\omega_m; i\nu_n).$$

(8)

Performing the sums on $n$ and $m$ in equation (8) finally leads to the appealing result

$$\chi_q^{tJ}(i\nu_n) = \chi_q^{HM}(i\nu_n) + J_q\chi_q^{HM}(i\nu_n)\chi_q^{tJ}(i\nu_n)$$

$$\chi_q^{tJ}(i\nu_n) = \chi_q^{HM}(i\nu_n) \left[ 1 - J_q\chi_q^{HM}(i\nu_n) \right]^{-1}$$

(9)

as expression for the magnetic susceptibility of the $t$-$J$ model in the DMFT. Thus the major ingredient in the susceptibility of the $t$-$J$ model is the corresponding quantity of the HM for $U = \infty$. One should also note that the expression (9) is very similar to the standard RPA result

$$\chi_q(i\nu_n; U = 0) = \chi_q(i\nu_n; U = 0, J = 0) \left[ 1 - J_q\chi_q(i\nu_n; U = 0, J = 0) \right]^{-1}$$

(10)

for the corresponding noninteracting system. Thus, as far as the DMFT for the $t$-$J$ model is concerned, the susceptibility is formally obtained by simply replacing $\chi_q(i\nu_n; U = 0, J = 0)$ by $\chi_q(i\nu_n; U = \infty, J = 0)$ in the RPA-formulas. Let us emphasize
that this correspondence holds only on a formal level: The physical situation described
by (3) is of course fundamentally different from the one modeled by (14)!

2.2 The spin susceptibility of the Hubbard model

As already mentioned, the dynamic spin susceptibility of the Hubbard model in real
space is within the DMFT given by \[22\]

\[
\begin{align*}
\chi_{ij}^{HM}(i\omega_n, i\omega_m; i\nu_n) &= \beta\chi_{ij}^{(0)}(i\omega_n; i\nu_n)\delta_{nm} \\
&+ \frac{1}{\beta} \sum_{i, \omega_p} \chi_{il}^{(0)}(i\omega_n; i\nu_n) \Gamma_{il}^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_n) \chi_{lj}^{HM}(i\omega_p, i\omega_m; i\nu_n) .
\end{align*}
\]

Equation (11) obviously also holds for the local susceptibility, i.e.

\[
\chi_{\text{loc}}(i\omega_n, i\omega_m; i\nu_l) = \chi_{\text{loc}}^{(0)}(i\omega_n; i\nu_l) \left[ \beta\delta_{n,m} + \frac{1}{\beta} \sum_{i, \omega_p} \Gamma_{il}^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_l) \chi_{\text{loc}}(i\omega_p, i\omega_m; i\nu_l) \right] 
\]

(12)

with the same \(\Gamma_{il}^{\uparrow\downarrow}(i\omega_n, i\omega_p; i\nu_l)\) as in equation (11). Combining equations (7) and (12), the susceptibility can be expressed by the local susceptibility through a matrix equation

\[
\begin{align*}
\chi_{q,l}^{\uparrow}(i\omega_n, i\omega_m; i\nu_l) &= A_{q}(i\omega_n, i\omega_m; i\nu_l) \\
\Gamma_{q,l}^{\text{eff}} &= - \left( \chi_{q,l}^{(0)} \right)^{-1} - \left( \chi_{\text{loc},l}^{(0)} \right)^{-1} 
\end{align*}
\]

(13)

With the definition \([\Lambda_{q}]_m = \Lambda_i(i\omega_m) = \frac{1}{\beta} \sum_n \chi_{\text{loc}}(i\omega_n, i\omega_m; i\nu_l)\) and the symmetry relation \(\chi_{\text{loc}}(i\omega_n, i\omega_m; i\nu_l) = \chi_{\text{loc}}(i\omega_m, i\omega_n; -i\nu_l)\) following from the definition (3) we can...
formally perform the frequency sums in (13) to obtain

\[ \chi^{HM}_q(i\nu_l) = \chi^{HM}_{loc}(i\nu_l) + \frac{1}{\beta} \vec{N}^T \cdot \vec{\Gamma}^{eff}_{q,l} \cdot \vec{N}_{l} = \frac{1}{\beta} \chi^{HM}_{loc,l} \cdot \vec{\Gamma}^{eff}_{q,l} \cdot \vec{N}_{l} \tag{14} \]

as the final result for the magnetic susceptibility of the Hubbard model in the framework of the dynamical molecular field theory.

It is important to note that until now no explicit reference to the value of \( U \) has been made, i.e. equation (14) is valid for all \( U \). The form (14) for the susceptibility of the HM is especially convenient for computational reasons, because the outer sums on Matsubara frequencies have been performed exactly. These can pose numerical problems because \([\chi^{**}]_{nm}\) decays at most like \( 1/(nm) \) for large \( n, m \) and one has to care for the correct time ordering in the final sums (cf. equations (6) and (11)). Whereas for the inner sums the products occurring there lead to an asymptotic behaviour like at least \( \sim 1/n^2 \) and thus a well defined sum.

### 2.3 The local spin susceptibility

The only unknown quantity in equation (14) is the local susceptibility \( \chi_{loc}(i\omega_n, i\omega_m; i\nu_n) \) defined by

\[ \chi_{loc}(i\omega_n, i\omega_m; i\nu_n) = \frac{1}{\beta} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 e^{-i\omega_n(\tau_1-\tau_2)} e^{-i\omega_m(\tau_3-\tau_4)} e^{-i\nu_n(\tau_2-\tau_4)} < T_e c_{i\uparrow}^\dagger(\tau_4) c_{i\downarrow}^\dagger(\tau_3) c_{i\downarrow}(\tau_2) c_{i\uparrow}(\tau_1) > \tag{15} \]

Within the DMFT, this function is obtained from the corresponding quantity of an effective SIAM with the band electrons replaced by the effective medium of the DMFT.
For finite $U$, the most successful way to solve the effective single-site problem and calculate functions like (15) is by Quantum Monte Carlo techniques [22]. However, since we are interested in the limit $U = \infty$ in the current context, this technique is not available. On the other hand, for $U = \infty$ the time-ordered perturbation theory [26] provides a natural and easy access to local quantities. In this method one expresses all local quantities through the resolvents $P_{0(1\sigma)}(z)$ of the unoccupied (occupied) ionic states. Of course, this theory cannot be solved exactly, so further approximations have to be introduced. Here, we shall use the so-called non-crossing approximation (NCA) [26,27] to calculate these resolvents and express further local correlation functions of interest. In previous publications we have already shown that the NCA provides a reliable approximation scheme to calculate such local quantities [14,22,24]. Applying the standard diagrammatic rules of this perturbational technique [26] in conjunction with the NCA we obtain

$$
\chi_{\text{loc}}(i\omega_n, i\omega_m; i\nu_l) = -\frac{1}{Z_{\text{loc}}} \oint_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} P_1(z) P_1(z - i\nu_l) P_0(z - i\omega_n) P_0(z - i\omega_m - i\nu_l) \ (16)
$$

for the local susceptibility. In equation (16), $Z_{\text{loc}} = \sum_M \oint_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} P_M(z)$ denotes the local contribution to the partition function and the contour $\mathcal{C}$ surrounds all singularities of the integrands counterclockwise.

### 3 Results
3.1 General remarks

The expressions (14) and (16) in principle still allow for the calculation of the dynamical susceptibility. Unfortunately, the derivation of equation (14) utilizes the representation of all quantities in Matsubara-space, i.e. one would be left with the awkward task to analytically continue the results to the real axis. This nontrivial problem is left for a future publication [28]. In this contribution we will concentrate on the static susceptibility, i.e. we set $i\nu_l = 0$.

Before we turn to the actual results for the $U = \infty$-Hubbard and $t$-$J$ model let us first briefly discuss the special limit $\langle n \rangle = 1$. In this case the model (1) becomes equivalent to the Heisenberg model and it is a straightforward task to calculate the molecular field expression for the static susceptibility, which reads

$$\chi_{\vec{q}}^{\langle n \rangle = 1} = \frac{\beta}{1 - J_\alpha \frac{\beta}{2}}.$$  

(17)

Comparing this expression with the result for the $t$-$J$ model in equation (9), one sees that obviously $\chi_{\vec{q}}^{HM} \rightarrow \frac{\beta}{2}$ for $\langle n \rangle \rightarrow 1$. On the other hand, $\beta/2$ is also exactly the value we expect for the local susceptibility in this limit, i.e. $\chi_{loc}^{HM} \rightarrow \frac{\beta}{2}$ for $\langle n \rangle \rightarrow 1$. From this it at once follows that the second part in equation (14) will become negligible for $\langle n \rangle$ close to half filling. On the one hand this offers a rather sensible test for the numerics involved in calculating the susceptibility for the HM. In addition it provides an interesting approximate ansatz for the susceptibility of the $t$-$J$ model by setting $\chi_{\vec{q}}^{HM} \approx \chi_{loc}^{HM}$ in this limit. Note that this also allows for a simple approximate calculation of dynamics since $\chi_{loc}^{HM}(\omega)$ is much easier to obtain than $\chi_{\vec{q}}^{HM}(\omega)$ given by
The latter observation is especially interesting in the light of recent studies by Scalapino et al. who analyzed the dynamical susceptibility for the twodimensional $t$-$J$ model obtained from exact diagonalization and found that it was rather well described by a form like (9) with $\chi_H^M(\omega)$ replaced by some local quantity [29].

3.2 The Hubbard model

Let us start by discussing the Lindhardt function

$$\chi(0)_{\vec{q}} = \frac{1}{N\beta} \sum_{\omega_n, \vec{k}} G_{\vec{k}+\vec{q}}(i\omega_n)G_{\vec{k}}(i\omega_n) .$$  (18)

While the whole derivation was completely independent of the actual lattice structure, we now have to specify the meaning of the $\vec{k}$-sum. We here choose a simple cubic lattice in $d$ dimensions, i.e. the coordination number is $Z = 2d$, and take the limit $d \to \infty$ to use the simplifications arising in this limit [19]. With $t^* = 1$ as the unit of energy, one then obtains for the single-particle DOS the well-known Gaussian form $\rho_0(\epsilon) = \exp(-\epsilon^2)/\sqrt{\pi}$ [19] and one can also evaluate the $\vec{k}$-sum in equation (18) analytically [19,20] to yield

$$\chi(0)_{\vec{q}} = \frac{1}{\beta} \sum_{\omega_n} \int_{-\infty}^{\infty} d\epsilon d\epsilon' \frac{\rho_0(\epsilon)\rho_0(\epsilon')}{(i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon) \cdot (i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon - \eta_{\vec{q}} - \epsilon' \cdot \sqrt{1 - \eta_{\vec{q}}^2})} .$$  (19)

In relation (19), $\eta_{\vec{q}} = \sum_{l=1}^{d} \cos(q_l \cdot a)/d$ and $\Sigma(z)$ is the one-particle self energy of the HM for a given $U \geq 0$. Note that the external wave-vector $\vec{q}$ only enters via the function $\eta_{\vec{q}}$ which basically describes surfaces of constant energy in the simple cubic Brillouin zone. For presentational reasons, we shall choose the special vector $\vec{q} = q(1,1,1,1,\ldots)$.
and use the number \( q \) with \( 0 \leq q \leq \pi \) as label rather than \(-1 \leq \eta_{q} \leq 1\).

![Figure 1: Lindhardt function for \( U = 0, 4, 7 \) and \( U = \infty \)](image)

The Lindhardt function for the HM for four different values of \( U = 0, 4, 7 \) and \( U = \infty \) at a filling \( \langle n \rangle = 0.95 \) and for a low temperature \( T = 1/30 \) is shown in Fig. [1].

Note the different scales for \( U = 0 \) (right scale) and \( U = 4, 7 \) and \( U = \infty \) (left scale)!

Without looking at the details it is thus clear, that the correlations induced by \( U \) strongly suppress this quantity. In addition one can observe a dramatic change in the \( q \)-dependence with increasing \( U \). While for \( U = 0 \) one has a strong peak at \( q = \pi \) due to the nesting property of the simple-cubic Fermi surface close to half filling this feature is strongly suppressed by the damping introduced by the correlations for \( U = 4, 7 \) and \( U = \infty \). In addition there occurs a cross-over from the maximum in \( \chi^{(q)}_{0} \) being at \( q = \pi \) for small \( U \) to \( q = 0 \) for \( U = \infty \). Note also that in contrast to \( U = 0 \) the total
$q$-dependence is rather weak in the other cases.

From the previous observation one may deduce two things: First, since for $U = \infty$ there is no net magnetic exchange between neighbouring sites, we expect from the flatness of $\chi_{\vec{q}}^{(0)}$ that also $\chi_{\vec{q}}^{HM}$ will be relatively flat as a function of $\vec{q}$. In addition, the fact that $\chi_{\vec{q}}^{(0)}$ is maximal at $q = 0$ suggests that $\chi_{\vec{q}}^{HM}$ for $U = \infty$ will be enhanced at $q = 0$ rather than at $q \approx \pi$ as expected and observed for $U < \infty$ [22].

\begin{figure}
\centering
\includegraphics[width=\textwidth]{susceptibility.png}
\caption{Susceptibility of the HM at $U = \infty$ as function of $\vec{q}$ and filling for two different temperatures $T = 1/5$ and $T = 1/40$.}
\end{figure}

This behaviour can indeed be seen in Fig. 2, where we have plotted $\chi_{\vec{q}}^{HM}$ for two different temperatures as function of $q$ and doping $\delta = 1 - \langle n \rangle$. The susceptibility was normalized to its value at $\delta = 0$, i.e. to $\chi_{\vec{q}}^{HM}(\delta = 0) = \beta/2$. Note that we always find $\chi_{\vec{q}}^{HM}(\delta > 0) < \chi_{\vec{q}}^{HM}(\delta = 0)$. From the form (3) for the susceptibility of the $t$-$J$ model it then at once follows that also $\chi_{\vec{q}}^{tJ}(\delta > 0) < \chi_{\vec{q}}^{tJ}(\delta = 0)$ for all values of $J^*$ and $\vec{q}$. This should be compared with results from high-temperature expansions for $d = 2$ [11].
which suggest a pronounced maximum in the uniform susceptibility around \( \delta = 15\% \) produced by spin fluctuations not included in the current mean-field treatment.

Another interesting feature in Fig. 2 is that in all cases the variation with \( q \) is comparatively weak, becoming somewhat stronger for lower temperatures and with increasing doping \( \delta \). We also observe a slight maximum at \( q = 0 \) that becomes more pronounced for lower temperatures but interestingly weakens with decreasing doping for \( T \) fixed. This observation is substantiated by a look at the doping dependence of \( \chi_{q}^{HM} \) in Fig. 3 for the local (circles), ferromagnetic \( q = 0 \) (squares) and antiferromagnetic \( q = \pi \) (diamonds) susceptibility for an inverse temperature \( \beta = 30 \). It is interesting to note that the antiferromagnetic susceptibility of the HM at \( U = \infty \) is always very close to the local one, which can be understood by the fact that due to the mapping of the HM onto an equivalent impurity model the local susceptibility already contains most of the (nearest-neighbour) antiferromagnetic correlations. Since for \( U = \infty \) there is no additional net magnetic exchange the nonlocal corrections only give a small renormalization. In contrast to this the renormalizations for the ferromagnetic susceptibility are comparatively strong and definitely tend to enhance this quantity above both the local and antiferromagnetic susceptibility. These results have to be interpreted in the light of Nagaoka’s theorem \[30\], where in the presence of one hole a ferromagnetic state for the background is favoured from a minimization of the hopping energy in the correlated system but not as a result of a direct magnetic coupling. Obviously, our results suggest that sizeable ferromagnetic correlations still exist for a finite number of holes. However, so far we do not find any hint towards a ferro-
magnetic instability at low temperatures close to half filling. This is consistent with the conjecture that for bipartite lattices – like the simple hyper-cubic lattice studied here – the critical hole density for the Nagaoka state should be $\delta_c = 0$ [31].

3.3 Results for the $t$-$J$ model

Inserting the results for the susceptibility of the HM at $U = \infty$ into equation (8) we obtain the susceptibility for the $t$-$J$ model as function of $q$ and $J^*$ as shown in Fig. 4 for $\langle n \rangle = 0.95$ and $\beta = 30$. The explicit exchange now obviously favours the antiferromagnetic point $q = \pi$ and eventually leads to an antiferromagnetically ordered state for $J^* > J^*_c \approx 0.085$ for this particular parameter set.

The temperature dependence of $1/\chi_{AF}^{tJ}$ for a specific value of $J^* = 0.067$ and three
Figure 4: Susceptibility of the $t$-$J$ model as function of $\vec{q}$ for various values of $J$ at a doping $\delta = 5\%$ and $\beta = 30$.

dopings $\delta = 2\%$, $\delta = 9\%$ and $\delta = 15\%$ is collected in Fig. 5. The full curve marks for comparison the case $\delta = 0$, where one has exactly $1/\chi_{\text{AF}}^{tJ} = 2 \cdot (T - J^*/2)$. As expected for a mean-field theory, close to the antiferromagnetic transition one finds a behaviour $1/\chi_{\text{AF}}^{tJ} = (T - T_N)/C_{\text{eff}}$ in all cases with decreasing Néel temperature $T_N$ and decreasing effective Curie constant $C_{\text{eff}}$ for increasing $\delta$ (see e.g. inset to Fig. 5).

It is quite noteworthy that close to half filling (i.e. for $\delta = 2\%$) this linearity extends up to rather high temperatures. However, with increasing doping one eventually finds appreciable deviations from this linearity for temperatures well above $T_N$. Both $T_N$ and $C_{\text{eff}}$ vary roughly linear up to 15% doping. We would also like to point out that
Figure 5: Inverse susceptibility of the t-J model as function of $T$ for $J^* = 0.067$ and three dopings $\delta = 2\%$, $\delta = 9\%$ and $\delta = 15\%$. Close to the phase transition one observes $\chi_{AF}^{-1}(T) = (T - T_N)/C_{eff}$ as expected for a mean-field theory. Note that for $\delta \to 0$ the linear behaviour is observed up to $T = 1t^*$. The full line represents half filling, where $\chi_{AF}^{-1} = 2 \cdot (T - J^*/2)$. The inset shows the dependence of the Néel temperature $T_N$ and effective Curie constant $C_{eff}$ on $\delta$. Up to a doping of $\delta = 15\%$ we do not observe any tendency towards incommensurate order.

With the method outlined above we are now able to calculate the phase diagram $T_N(\delta, J^*)$ for the t-J model. The results for dopings $\delta \leq 15\%$ and $J^* < 0.12$ are shown in Fig. 6. One observes the expected increase in the Néel temperature $T_N$ with...
Figure 6: Phase diagram $T_N(\delta, J)$ for the $t$-$J$ model. The dashed lines represent (linear) extrapolations of the phase boundaries to $T = 0$. The corresponding values of $J_c(\delta)$ behave like $J_c(\delta) \sim \delta^2$, as shown in the inset.

Increasing $J^*$ and a – for larger $\delta$ roughly linear – decrease as function of $\delta$. We may use this approximate linearity of $T_N(\delta)$ to extrapolate the curves $T_N(\delta)$ for a given $J^*$ to $T = 0$. This procedure allows us to obtain an extrapolation for the phase diagram $J^*_c(\delta)$ of the $t$-$J$ model at $T = 0$. The result is shown in the inset to Fig. 6. We find that $J^*_c(\delta)$ behaves rather accurately like $J^*_c \sim \delta^2$. The phase diagram in Fig. 6 should be compared to the DMFT results for the Hubbard model in the strong coupling limit [32].
In reference [32] the authors calculate $T_N(\delta, U)$ up to $U = 7t^*$, which would correspond to $J^* \approx 0.14$ for the $t$-$J$ model. They also observe an almost linear dependence of $T_N$ on the doping $\delta$ for large values of $U$. However, although the value of $T_N$ for $\delta \rightarrow 0$ and the observed linearity agrees quite well with our results, the depression of $T_N$ as function of $\delta$ for the Hubbard model at $U = 7t^*$ is much faster than in our Fig. 3. In addition one encounters a transition into an incommensurate state for $\delta \gtrsim 12\%$ in the Hubbard model. Currently it is not clear whether these deviations – especially the lack of an incommensurate magnetic order for large doping – between the results for the large-$U$ Hubbard model and the $t$-$J$ model are real or due to the additional approximations introduced by using the NCA to solve the effective impurity problem. One should keep in mind, though, that for finite $U$ respectively $J^*$ the Hubbard model and the $t$-$J$ model are expected to show different physical behaviour: The mapping of the Hubbard model to an effective model with magnetic exchange generates in addition to the exchange term included in the $t$-$J$ model also more complicated couplings, like for instance a three-site term which is also of the order $J^*$ [5] and may give rise to quite important corrections in physical quantities [33].

Finally we should like to use the observation that close to half filling the susceptibility for the HM is relatively flat with respect to $\vec{q}$ and obtain an approximation for the dynamical spin structure factor $S(\vec{q}, \omega) = \Im m \chi(\omega)/(1 - e^{-\beta \omega})$ by assuming $\chi^{HM}(\omega) \approx \chi^{HM}_{loc}(\omega)$ in equation (9). This approximation avoids the cumbersome calculation of the $\vec{q}$-dependent susceptibility for finite frequencies. As an example the result for $J^* = 0.035$, $T = 1/30$ and $\delta = 5\%$ is shown in Fig. 4. As expected, the
Figure 7: Approximate result for $S_{q}^{IJ}(\omega)$ for $\delta = 5\%$, $T = 1/30$ and $J = 0.035$.

maximum in $S_{q}^{IJ}(\omega)$ is found at $q = \pi$ and $\omega = 0$ and the intensity decays very fast with increasing energy for all $\vec{q}$. Since this quantity or its value at $q = \pi$ and $\omega = 0$ can be measured by neutron scattering or NMR relaxation [34], it is definitely necessary to study the dependence on doping, temperature and $J^*$ more systematically. This is left for a future publication.
4 Summary and outlook

We presented a theory and results for the magnetic properties of the $t$-$J$ model in the framework of the dynamical mean-field theory, which treats both the correlated hopping of the fermionic degrees of freedom and the nonlocal exchange coupling between the spin degrees of freedom on the same footing. As has been pointed out [21], this approach ensures a thermodynamically consistent description of the properties of the system and especially does not introduce artificial phase transitions like e.g. in slave-boson mean field theories.

One in our opinion particularly interesting result is that the dynamical susceptibility of the $t$-$J$ model can be expressed in an RPA-like fashion by the susceptibility of the Hubbard model at $U = \infty$ (cf. equation (3)). In addition the latter can be split into a local part plus a $\vec{q}$-dependent renormalization which for low doping turned out to be relatively small and only moderately varying with $\vec{q}$. We find that in the case $J^* = 0$ (i.e. $U = \infty$) the absence of an explicit magnetic exchange leads to $\chi_{q=\pi}^{HM} \approx \chi_{loc}^{HM}$ and an interesting enhancement of the ferromagnetic correlations. This is in contrast to the HM at finite $U$, where the effective magnetic exchange $J \sim t^2/U$ leads to a strongly enhanced susceptibility at $q = \pi$ and a suppression at $q = 0$ instead. However, for the situation considered here – simple hypercubic lattice with nearest-neighbour hopping only – we did not observe a tendency towards a magnetic instability at $q = 0$ for finite doping, in accordance with results obtained by other groups. The occurrence of an enhanced ferromagnetic susceptibility for Hubbard model in the limit $U = \infty$
nevertheless motivates a more detailed investigation of the mean-field properties of the Hubbard model in this particular limit for different lattice structures and longer-range hopping.

A finite magnetic exchange $J^*$ again strongly enhances the antiferromagnetic susceptibility. When one further increases $J^*$ one eventually encounters a phase transition into an antiferromagnetic phase at a critical value $J^*_c(T, \delta)$. From our results of $\chi_{AF}^H(T, \delta)$ we extracted the phase diagram $T_N(\delta, J^*)$. We found that $T_N$ increases monotonically as function of $J^*$ and – for fixed $J^*$ – decreases monotonically as function of $\delta$. For larger doping $\delta$ we observed that the curves $T_N(\delta)$ for different but fixed values of $J^*$ are almost linear. This linearity agrees at least qualitatively with DMFT results for the Hubbard model at finite $U$, where one finds a crossover from standard weak-coupling behaviour in $T_N(\delta)$ for small $U$ to an almost linear variation for $U \geq 7t^*$. However, in contrast to our results one observes a much faster depression of $T_N$ as function of $\delta$ and in addition a transition into an incommensurate phase for large $\delta$. Especially the latter feature was not reproduced in our calculations. The linearity of $T_N(\delta)$ finally allowed us to extrapolate our data to obtain an approximation for the magnetic phase boundary of the $t$-$J$ model at $T = 0$.

The relatively weak dependence of the susceptibility of the HM on $\vec{q}$ was used to set up an approximation for the dynamical susceptibility by assuming $\chi_{\vec{q}}^H(\omega) \approx \chi_{\text{loc}}^H(\omega)$, thus giving to some extent a microscopic justification of the results in reference [29]. Since in addition $\chi_{\text{loc}}^H(\omega)$ can be calculated fairly easy from the effective single-site
problem we were able to present results for the dynamical spin structure factor $S_{\vec{q}}^{tJ}(\omega)$.

The general expected features, i.e. sharp maximum at $q = \pi$ and $\omega = 0$, a shift of the maximum to finite $\omega$ for $q < \pi$ and a fast decay as $\omega > 0$, are well reproduced. There are of course several questions left. First of all one should check the assumption of a nearly $\vec{q}$-independent $\chi_{\vec{q}}^{HM}(\omega)$ carefully for several values of doping and temperature. Second a systematic study of $S_{\vec{q}}^{tJ}(\omega)$ as function of doping and temperature is clearly needed. Another important issue not yet addressed concerns phase separation in the $t$-$J$ model, which among other problems requires e.g. the evaluation of the compressibility in the antiferromagnetic phase. Work along this line is in progress.

Finally, one should stress again that the results presented here were calculated with a generalized mean-field theory or equivalently for the limit $d = \infty$. This obviously means that their applicability to e.g. the $t$-$J$ model in $d = 2$ or $d = 3$ is unclear. From high-temperature expansions or exact diagonalizations for $d = 2$ one knows for example that the static homogenous susceptibility shows a nonmonotonic behaviour as function of $\delta$, which may be attributed to fluctuations induced by the spin-flip term in the model (1). Since the DMFT neglects this type of processes it is not too surprising that in our results we always observe a monotonic decrease instead. We thus do expect that the predictions of the DMFT will be modified not only quantitatively but most likely also qualitatively, especially for two-dimensional systems.

**Acknowledgements:** We like to acknowledge useful discussions with D. Vollhardt, M. Jarrell, W. Metzner, F. Gebhardt, P. van Dongen, G. Uhrig, K. Becker, N. Grewe, F. Anders, and many others. This work was supported by the Deutsche Forschungsge-
meinschaft grant number Pr 298/3-1.

One of us (TP) also wants to acknowledge the hospitality of the department of physics at the University of Cincinnati, where part of this work was done.

References

[a] Permanent address: Angoss Software International, Toronto, Ontario, Canada M5V 1J5.

[1] P.W. Anderson, Phys. Rev. 124, 41(1961).

[2] N. Grewe und F. Steglich. Heavy fermions. In K.G. Gschneidner Jr., K.A. Eyring (eds.), Handbook of the Physics und Chemistry of Rare-Earths Vol. 14. (North-Holland Publ. Co., 1991, Amsterdam).

[3] J. Hubbard, Proc. R. Soc. a276, 238(1963); M.C. Gutzwiller, Phys. Rev. Lett. 10, 159(1963); J. Kanamori, Prog. Theor. Phys. 30, 257(1963).

[4] P.W. Anderson, Science 235, 1196(1987).

[5] P.W. Anderson, Solid State Phys. 14, 99(1963); L.N. Bulaevskii, E.L. Nagaev und D.I. Khomskii, Zh. Eksp. Teor. Fiz 54, 1562(1968) (Sov. Phys. – JETP 27, 836(1968)); K.A. Chao, J. Spalek and A.M. Oleś, J. Phys. C 10, L271(1977); C. Gros, R. Joynt and T.M. Rice, Phys. Rev. B36, 381(1987); H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 57, 2482(1988).
[6] J. Hubbard, Proc. Roy. Soc. A281, 401(1964).

[7] E.H. Lieb and F.Y. Wu, Phys. Rev. Lett., 20, 1445(1968).

[8] P. Schlottmann, Phys. Rev. B36, 5117(1987); N. Kawakami and S.-K. Yang, Phys. Rev. Lett. 65, 2309(1990).

[9] M. Ogata, M. Luchini, S. Sorella and F. Assaad, Phys. Rev. Lett. 66, 2388(1991).

[10] Th. Pruschke and H. Shiba, Phys. Rev. B46, 356(1992); Th. Pruschke and H. Shiba, Physica C 185-189, 1573(1991).

[11] W.O. Puttika, M.U. Luchini and T.M. Rice, Phys. Rev. Lett. 68, 538(1992); R.R.P. Singh and R.L. Glenister, Phys. Rev. B46, 11871(1992).

[12] For a recent review see: E. Dagotto, Rev. Mod. Phys. 66, 763(1994).

[13] J. Jaklič and P. Prelovšek, Phys. Rev. B49, 5065(1994); Phys. Rev. B50, 7129(1994); Phys. Rev. Lett. 75, 1340(1995).

[14] Th. Pruschke, M. Jarrell and J.K. Freericks, to appear in Adv. Phys.

[15] R. Preuss, W. Hanke und W. von der Linden, Phys. Rev. Lett. 75, 1344(1995).

[16] Th. Obermeier, Th. Pruschke and J. Keller, submitted to Annalen der Physik.

[17] E. Arrigoni, C. Castellani, M. Grilli, R. Raimondi, G.C. Strinati, Physics Reports 241, 291(1994); E. Arrigoni, G.C. Strinati, Phys. Rev. B52, 2428(1995).

[18] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324(1989).
[19] E. Müller-Hartmann, Z. Phys. B\textbf{74}, 507(1989).

[20] U. Brandt, C. Mielsch, Z. Phys. B \textbf{75}, 365 (1989).

[21] V. Janiš, Z. Phys. B\textbf{83}, 227(1991); V. Janiš and D. Vollhardt, Int. J. Mod. Phys. B \textbf{6}, 731(1992).

[22] M. Jarrell, Phys. Rev. Lett. \textbf{69}, 168 (1992); M. Jarrell, T. Pruschke, Z. Phys. B \textbf{90}, 187 (1993).

[23] A. Georges and G. Kotliar, Phys. Rev. B\textbf{45}, 6479(1992); A. Georges, G. Kotliar and Q. Si, Int. J. Mod. Phys. B\textbf{6}, 705(1992).

[24] Th. Pruschke, D.L. Cox and M. Jarrell, Phys. Rev. B\textbf{47}, 3553(1993).

[25] C. Itzykson and J.M. Drouffe, \textit{Statistical Field Theory}, Vol. I & II (Cambridge University Press 1989).

[26] H. Keiter, J.C. Kimball: Int. J. Magn. \textbf{1}, 233 (1971); N.Grewe, H.Keiter: Phys. Rev. B\textbf{24}, 4420 (1981); H. Keiter, G. Morandi: Phys. Rep. \textbf{109}, 227 (1984).

[27] N.E. Bickers, D.L. Cox and J.W. Wilkins, Phys. Rev. B\textbf{36}, 2036(1987)

[28] Th. Pruschke and Th. Obermeier, to be published.

[29] P. Monthoux and D. Pines, Phys. Rev. B\textbf{49}, 4261(1994); P. Monthoux und D.J. Scalapino, Phys. Rev. Lett. \textbf{72}, 1874(1994).

[30] Y. Nagaoka, Phys. Rev. \textbf{147}, 392(1966).
[31] P. Fazekas, B. Menge, and E. Müller-Hartmann, Z. Phys. B 78, 69 (1990); R. Strack und D. Vollhardt, Jou. of Low Temp. Physics 99, 385(1995).

[32] J.K. Freericks and M. Jarrell, Phys. Rev. Lett. 74, 186(1995).

[33] M. Ogata and H. Shiba, Phys. Rev. B 41, 2326(1990).

[34] T. Imai, C.P. Slichter, K. Yoshimura and K. Kasuge, Phys. Rev. Lett. 70, 1002(1993).