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1996 J. Phys.: Condens. Matter 8 3161

(http://iopscience.iop.org/0953-8984/8/18/009)

J. Phys.: Condens. Matter **8** (1996) 3161–3175. Printed in the UK

Magnetic properties of the *t–J* model in the dynamical mean-field theory

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Received 14 December 1995

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 nonlocal 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.

1. Introduction and survey

The description of strongly correlated electron systems involves by and large three different classes of model. 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 modelled 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-metal compounds like V_2O_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 for describing the properties of the cuprate superconductors. It is this model that 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, the two models are expected to differ fundamentally for increasing exchange interaction.

The Hamiltonian of the *t–J* model reads

$$H_{t-J} = -\frac{t^*}{\sqrt{2\mathcal{Z}}} \sum_{\langle ij\rangle\sigma} X^{(i)}_{1\sigma,0} X^{(j)}_{0,1\sigma} + \frac{J^*}{\mathcal{Z}} \sum_{\langle ij\rangle} \boldsymbol{S}^i \cdot \boldsymbol{S}^j. \tag{1}$$

In equation (1), $X^{(j)}_{MM'} = |j, M\rangle\langle j, M'|$ are the standard Hubbard operators [6] 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 $\boldsymbol{S}^i$ denotes the spin operator on site i. The sums in the Hamiltonian (1)

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0953-8984/96/183161+15$19.50

are over nearest neighbours only. The transfer and exchange integrals t and J have been rescaled with the coordination number $\mathcal{Z}$ of the system to guarantee a physically 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 for $d = 1$ except for at the two special points $J^* = 0$ (the Hubbard model) [7] and $J^* = 2t^*$ (the supersymmetric t–J model) [8]. 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-rich and a hole-rich region [9]. Interestingly, close to this boundary, the ground state of the t–J model is dominated by superconducting pair correlations [10], 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 $J^*/t^* \sim 3$–4 for this scenario. The interesting question thus is how these features survive for $d > 1$ and especially to what extent phase separation might occur at much lower values of J, as suggested by, e.g., high-temperature expansions [11].

While for $d = 1$ the combination of exact diagonalization and tools of conformal field theory provides a powerful framework within which to extract information about the asymptotics of the macroscopic system, similar methods do not exist for $d > 1$. Quantum Monte Carlo techniques, too, cannot be applied for realistic lattice sizes and temperatures due to a severe minus-sign problem. Thus most information about the properties of the t–J model comes 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 the resolving of dynamically generated low-energy features, which one may especially expect close to half-filling [14–16]. 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 for obtaining results in the thermodynamic limit is needed.

Usually, mean-field theory provides a reliable tool for studying at least the qualitative features of models in theoretical solid-state physics. However, until recently a thermodynamically consistent mean-field theory, like that 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 has been introduced to define a thermodynamically consistent mean-field theory for correlated systems that preserves the local dynamics exactly [20–22]. 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 has been 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 [20–23]. 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 band states are replaced by an effective medium obtained from the full problem with the site under consideration removed [20–23]. The one-particle Green's 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 is no complete solution for the SIAM. However, there are at least different numerical exact techniques like quantum Monte Carlo and controlled perturbational approximations for solving this local model [14, 24]. All of 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 what is found from standard mean-field theory (like, e.g., that for the Heisenberg model) one obtains a complex, frequency-dependent function as the 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 $U = \infty$. Considering 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 [16].

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

$$\chi_{\boldsymbol{q}}^{t-J}(\mathrm{i}\nu_n) = \frac{1}{\beta^2} \sum_{\omega_n,\omega_m} \chi_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n) \mathrm{e}^{\mathrm{i}(\omega_n+\omega_m)0^+} \tag{2}$$

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

$$\chi_{ij}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l) = \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \int_0^\beta \mathrm{d}\tau_3 \int_0^\beta \mathrm{d}\tau_4 \; \mathrm{e}^{-\mathrm{i}\omega_m(\tau_1-\tau_2)} \mathrm{e}^{-\mathrm{i}\omega_n(\tau_3-\tau_4)} \mathrm{e}^{-\mathrm{i}\nu_l(\tau_2-\tau_4)}$$
$$\times \langle T_\tau c_{i\uparrow}(\tau_4) c_{i\downarrow}^+(\tau_3) c_{j\downarrow}(\tau_2) c_{j\uparrow}^+(\tau_1) \rangle_{t-J}. \tag{3}$$

In equations (2) and (3) $\mathrm{i}\omega_n$ and $\mathrm{i}\omega_m$ denote Fermi Matsubara frequencies and $\mathrm{i}\nu_n$ a Bose Matsubara frequency. Quite generally, by introducing the irreducible two-particle self-

energy $\Gamma^{\uparrow\downarrow}_{ij}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l)$, the particle–hole propagator (3) can formally be written as

$$\chi_{ij}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l) = \beta\chi^{(0)}_{ij}(\mathrm{i}\omega_n; \mathrm{i}\nu_l)\delta_{n,m} + \frac{1}{\beta}\sum_{lk,\mathrm{i}\omega_p} \chi^{(0)}_{il}(\mathrm{i}\omega_n; \mathrm{i}\nu_l)\Gamma^{\uparrow\downarrow}_{lk}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_l)\chi_{kj}(\mathrm{i}\omega_p, \mathrm{i}\omega_m; \mathrm{i}\nu_l). \tag{4}$$

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

Using standard techniques of field theory [20], one can express the irreducible particle–hole self-energy as a 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 at the Hartree level it follows that the two-particle self-energy acquires the particularly simple form

$$\Gamma^{\uparrow\downarrow}_{lk}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_l) = -\frac{J^*}{\mathcal{Z}}\delta_{|l-k|,\mathrm{n.N.}} + \Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_l)\delta_{lk}. \tag{5}$$

The nontrivial 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 $\boldsymbol{q}$-space, we obtain as the transverse magnetic susceptibility of the t–J model in the DMFT

$$\chi_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n) = \beta\chi^{(0)}_{\boldsymbol{q}}(\mathrm{i}\omega_n; \mathrm{i}\nu_n)\delta_{nm} + J_{\boldsymbol{q}}\chi^{(0)}_{\boldsymbol{q}}(\mathrm{i}\omega_n; \mathrm{i}\nu_n)\frac{1}{\beta}\sum_p \chi_{\boldsymbol{q}}(\mathrm{i}\omega_p, \mathrm{i}\omega_m; \mathrm{i}\nu_n) + \frac{1}{\beta}\sum_p \chi^{(0)}_{\boldsymbol{q}}(\mathrm{i}\omega_n; \mathrm{i}\nu_n)\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_n)\chi_{\boldsymbol{q}}(\mathrm{i}\omega_p, \mathrm{i}\omega_m; \mathrm{i}\nu_n). \tag{6}$$

In equation (6) $J_{\boldsymbol{q}}$ denotes the Fourier transform of $-(J^*/\mathcal{Z})\delta_{|i-j|,\mathrm{n.N.}}$. For the case of a simple hypercubic lattice one, e.g., obtains

$$J_{\boldsymbol{q}} = -\frac{J^*}{d}\sum_{l=1}^{d}\cos(q_l a).$$

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

$$\chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n) = \beta\chi^{(0)}_{\boldsymbol{q}}(\mathrm{i}\omega_n; \mathrm{i}\nu_n)\delta_{nm} + \frac{1}{\beta}\sum_p \chi^{(0)}_{\boldsymbol{q}}(\mathrm{i}\omega_n; \mathrm{i}\nu_n)\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_n)\chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\omega_p, \mathrm{i}\omega_m; \mathrm{i}\nu_n). \tag{7}$$

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

$$\chi_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n) = \chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n) + J_{\boldsymbol{q}}\frac{1}{\beta}\sum_l \chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_l; \mathrm{i}\nu_n)\frac{1}{\beta}\sum_p \chi_{\boldsymbol{q}}(\mathrm{i}\omega_p, \mathrm{i}\omega_m; \mathrm{i}\nu_n). \tag{8}$$

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

$$\begin{aligned}\chi^{t-J}_{\boldsymbol{q}}(\mathrm{i}\nu_n) &= \chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\nu_n) + J_{\boldsymbol{q}}\chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\nu_n)\chi^{t-J}_{\boldsymbol{q}}(\mathrm{i}\nu_n)\\ \chi^{t-J}_{\boldsymbol{q}}(\mathrm{i}\nu_n) &= \chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\nu_n)\left[1 - J_{\boldsymbol{q}}\chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\nu_n)\right]^{-1}\end{aligned} \tag{9}$$

as the 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 expression (9) is very similar to the standard RPA result

$$\chi_{\boldsymbol{q}}(\mathrm{i}\nu_n; U = 0) = \chi_{\boldsymbol{q}}(\mathrm{i}\nu_n; U = 0, J = 0)\left[1 - J_{\boldsymbol{q}}\chi_{\boldsymbol{q}}(\mathrm{i}\nu_n; U = 0, J = 0)\right]^{-1} \tag{10}$$

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 $\chi_{\boldsymbol{q}}(\mathrm{i}\nu_n; U = 0, J = 0)$ by $\chi_{\boldsymbol{q}}(\mathrm{i}\nu_n; U = \infty, J = 0)$ in the RPA formulas. Let us emphasize that this correspondence holds only on a formal level: the physical situation described by (9) is of course fundamentally different from the one modelled by (10)!

2.2. The spin susceptibility of the Hubbard model

As already mentioned, the dynamical spin susceptibility of the Hubbard model within the DMFT is given by equation (7) [22], with only $\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_n)$ being unknown. Usually, the direct calculation of quantities like $\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_n)$ is rather hopeless, especially for correlated electron systems.

At this point we can use one major aspect of the DMFT, namely that the whole system is described by an effective local problem [20–23]. We can of course calculate a spin susceptibility for this effective local problem, which obviously also has the general form (4) with all quantities being purely local by definition, i.e.

$$\chi_{loc}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l) = \chi^{(0)}_{loc}(\mathrm{i}\omega_n; \mathrm{i}\nu_l)\left[\beta\delta_{n,m} + \frac{1}{\beta}\sum_{\mathrm{i}\omega_p}\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_l)\chi_{loc}(\mathrm{i}\omega_p, \mathrm{i}\omega_m; \mathrm{i}\nu_l)\right] \tag{11}$$

with the same $\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_l)$ as in equation (7). The latter observation follows directly from the definition of $\Gamma^{\uparrow\downarrow}(\mathrm{i}\omega_n, \mathrm{i}\omega_p; \mathrm{i}\nu_l)$ and the locality of the one-particle self-energy [20].

Combining equations (7) and (11), the susceptibility can be expressed via the local susceptibility through a matrix equation ($[\mathbf{A}_{\boldsymbol{q},l}]_{nm} = A_{\boldsymbol{q}}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l)$):

$$\begin{aligned}\boldsymbol{\chi}_{\boldsymbol{q},l} &= \left[\overleftrightarrow{1} - \frac{1}{\beta}\boldsymbol{\chi}_{loc,l}\boldsymbol{\Gamma}^{eff}_{\boldsymbol{q},l}\right]^{-1}\boldsymbol{\chi}_{loc,l} \\ \boldsymbol{\Gamma}^{eff}_{\boldsymbol{q},l} &= -(\boldsymbol{\chi}^{(0)\,-1}_{\boldsymbol{q},l} - \boldsymbol{\chi}^{(0)\,-1}_{loc,l}).\end{aligned} \tag{12}$$

With the definition

$$[\boldsymbol{\Lambda}_l]_m = \Lambda_l(\mathrm{i}\omega_m) = \frac{1}{\beta}\sum_n \chi_{loc}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l)$$

and the symmetry relation $\chi_{loc}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l) = \chi_{loc}(\mathrm{i}\omega_m, \mathrm{i}\omega_n; -\mathrm{i}\nu_l)$ following from the definition (3) we can formally perform the frequency sums in (12) to obtain

$$\chi^{HM}_{\boldsymbol{q}}(\mathrm{i}\nu_l) = \chi_{loc}(\mathrm{i}\nu_l) + \frac{1}{\beta}\boldsymbol{\Lambda}^T_l\boldsymbol{\Gamma}^{eff}_{\boldsymbol{q},l}\frac{\overleftrightarrow{1}}{\overleftrightarrow{1} - (1/\beta)\boldsymbol{\chi}_{loc,l}\boldsymbol{\Gamma}^{eff}_{\boldsymbol{q},l}}\boldsymbol{\Lambda}_{-l} \tag{13}$$

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 (13) is valid for all U. The form (13) 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 $[\chi_{q,l}]_{nm}$ decays at most like $1/(nm)$ for large n, m and one has to exercise care regarding the correct time ordering in the final sums (cf. equations (6) and (7))—whereas for the inner sums the products occurring there lead to an asymptotic behaviour decaying at least like $1/n^2$ and thus a well defined sum.

2.3. The local spin susceptibility

The only unkown quantity in equation (13) is the local susceptibility $\chi_{loc}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n)$ defined by

$$\chi_{loc}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_n) = \frac{1}{\beta}\int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \int_0^\beta \mathrm{d}\tau_3 \int_0^\beta \mathrm{d}\tau_4\, \mathrm{e}^{-\mathrm{i}\omega_m(\tau_1-\tau_2)}\mathrm{e}^{-\mathrm{i}\omega_n(\tau_3-\tau_4)}\mathrm{e}^{-\mathrm{i}\nu_n(\tau_2-\tau_4)} \times \langle T_\tau c_{i\uparrow}(\tau_4)c^+_{i\downarrow}(\tau_3)c_{i\downarrow}(\tau_2)c^+_{i\uparrow}(\tau_1)\rangle. \tag{14}$$

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 (14) 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 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 noncrossing 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 for calculating such local quantities [14, 22, 24]. Applying the standard diagrammatic rules of this perturbational technique [26] in conjunction with the NCA we obtain

$$\chi_{loc}(\mathrm{i}\omega_n, \mathrm{i}\omega_m; \mathrm{i}\nu_l) = -\frac{1}{Z_{loc}}\oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\, \mathrm{e}^{-\beta z} P_1(z) P_1(z - \mathrm{i}\nu_l) P_0(z - \mathrm{i}\omega_n) P_0(z - \mathrm{i}\omega_m - \mathrm{i}\nu_l) \tag{15}$$

for the local susceptibility. In equation (15),

$$Z_{loc} = \sum_M \oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\, \mathrm{e}^{-\beta z} P_M(z)$$

denotes the local contribution to the partition function and the contour $\mathcal{C}$ surrounds all singularities of the integrands anticlockwise.

3. Results

3.1. General remarks

The expressions (13) and (15) in principle still allow for the calculation of the dynamical susceptibility. Unfortunately, the derivation of equation (13) utilizes the representation of all quantities in Matsubara space, i.e. one would be left with the awkward task of analytically continuing 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 $\mathrm{i}\nu_l = 0$.

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

$$\chi_q^{n=1} = \frac{\beta/2}{1 - J_q \beta/2}. \tag{16}$$

Comparing this expression with the result for the t–J model in equation (9), one sees that obviously $\chi_q^{HM} \to \beta/2$ for $\langle n \rangle \to 1$. On the other hand, $\beta/2$ is also exactly the value we expect for the *local* susceptibility in this limit, i.e. $\chi_{loc}^{HM} \to \beta/2$ for $\langle n \rangle \to 1$. From this it at once follows that the second part in equation (13) 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 obtained by setting $\chi_q^{HM} \approx \chi_{loc}^{HM}$ in this limit. Note that this also allows for a simple approximate calculation of the dynamics since $\chi_{loc}^{HM}(\omega)$ is much easier to obtain than $\chi_q^{HM}(\omega)$ given by (13). The latter observation is especially interesting in the light of recent studies by Scalapino *et al* who analysed the dynamical susceptibility for the two-dimensional t–J model obtained from exact diagonalization and found that it was rather well described by a form like (9) with $\chi_q^{HM}(\omega)$ replaced by some local quantity [29].

3.2. The Hubbard model

Let us start by discussing the Lindhardt function

$$\chi_q^{(0)} = -\frac{1}{N\beta} \sum_{\omega_n, \boldsymbol{k}} G_{\boldsymbol{k}+\boldsymbol{q}}(\mathrm{i}\omega_n) G_{\boldsymbol{k}}(\mathrm{i}\omega_n). \tag{17}$$

While the whole derivation was completely independent of the actual lattice structure, we now have to specify the meaning of the $\boldsymbol{k}$-sum. We here choose a simple cubic lattice in d dimensions, i.e. the coordination number is $\mathcal{Z} = 2d$, 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 $\boldsymbol{k}$-sum in equation (17) analytically [19, 20] to yield

$$\chi_q^{(0)} = \frac{1}{\beta} \sum_{\omega_n} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \; \mathrm{d}\epsilon' \; \frac{\rho_0(\epsilon)\rho_0(\epsilon')}{(\mathrm{i}\omega_n + \mu - \Sigma(\mathrm{i}\omega_n) - \epsilon)\left(\mathrm{i}\omega_n + \mu - \Sigma(\mathrm{i}\omega_n) - \epsilon\eta_{\boldsymbol{q}} - \epsilon'\sqrt{1 - \eta_q^2}\right)}. \tag{18}$$

In relation (18),

$$\eta_{\boldsymbol{q}} = \sum_{l=1}^{d} \cos(q_l a)/d$$

and $\Sigma(z)$ is the one-particle self-energy of the HM for a given $U \geqslant 0$. Note that the external wave-vector $\boldsymbol{q}$ only enters via the function $\eta_{\boldsymbol{q}}$ which basically describes surfaces of constant energy in the simple cubic Brillouin zone. For presentational reasons, we shall choose the special vector $\boldsymbol{q} = q(1, 1, 1, 1, \ldots)$ and use the number q with $0 \leqslant q \leqslant \pi$ as the label rather than $-1 \leqslant \eta_{\boldsymbol{q}} \leqslant 1$.

The Lindhardt functions for the HM for four different values of U, namely 0, 4, 7 and ∞, at a filling $\langle n \rangle = 0.95$ and for a low temperature $T = 1/30$ are shown in figure 1. Note

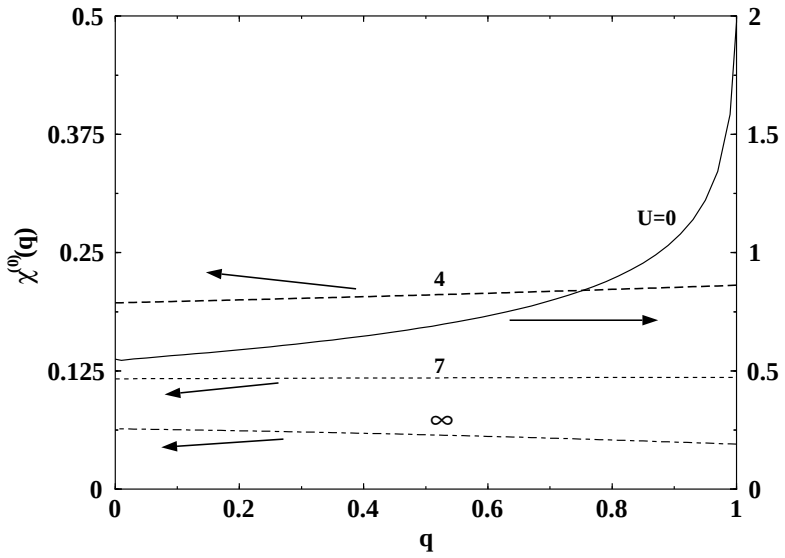

Figure 1. The Lindhardt functions for $U = 0$, 4, 7 and ∞.

the different scales for $U = 0$ (right-hand scale) and $U = 4$, 7 and ∞ (left-hand 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 ∞. In addition there occurs a crossover from the maximum in $\chi_q^{(0)}$ being at $q = \pi$ for small U to it being at $q = 0$ for $U = \infty$. Note also that in contrast to what is found when $U = 0$, 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 $\chi_q^{(0)}$ that also χ_q^{HM} will be relatively flat as a function of $\boldsymbol{q}$; in addition, the fact that $\chi_q^{(0)}$ is maximal at $q = 0$ suggests that χ_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].

This behaviour can indeed be seen in figure 2, where we have plotted the χ_q^{HM} for two different temperatures as functions of q and doping $\delta = 1 - \langle n \rangle$. The susceptibility was normalized to its value at $\delta = 0$, i.e. to $\chi_q^{HM}(\delta = 0) = \beta/2$. Note that we always find $\chi_q^{HM}(\delta > 0) < \chi_q^{HM}(\delta = 0)$. From the form (9) for the susceptibility of the t–J model it then at once follows that also $\chi_q^{t-J}(\delta > 0) < \chi_q^{t-J}(\delta = 0)$ for all values of J^* and $\boldsymbol{q}$. This should be compared with results from high-temperature expansions for $d = 2$ [11] which suggest a pronounced maximum in the uniform susceptibility at around $\delta = 15\%$ produced by spin fluctuations not included in the current mean-field treatment.

Another interesting feature in figure 2 is that in all cases the variation with q is comparatively weak, becoming somewhat stronger for lower temperatures and with increasing doping δ. 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 χ_q^{HM} in figure 3 for the local (circles), ferromagnetic $q = 0$ (squares) and antiferromagnetic $q = \pi$

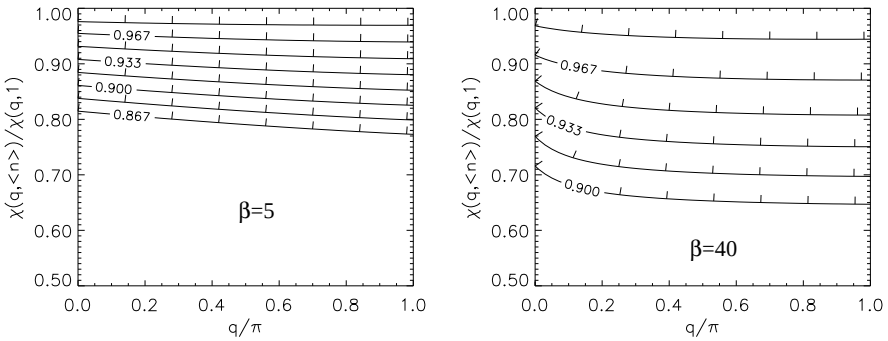

Figure 2. The susceptibility of the HM at $U = \infty$ as a function of $\boldsymbol{q}$ and filling for two different temperatures $T = 1/5$ and $T = 1/40$.

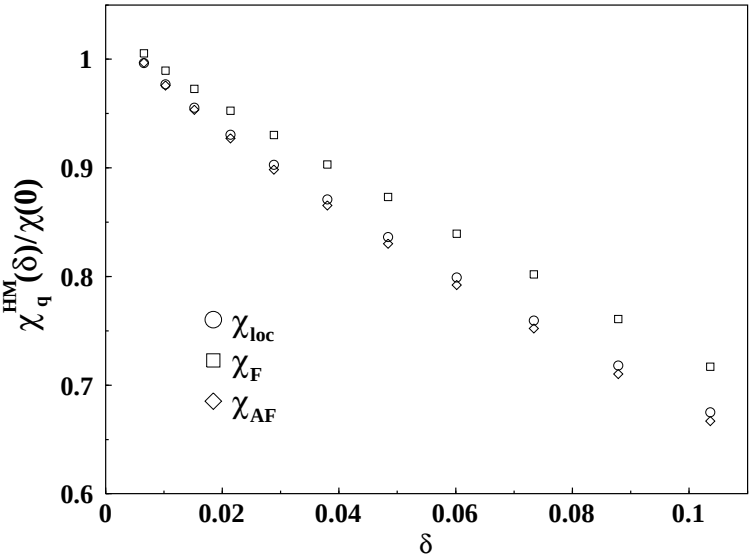

Figure 3. The susceptibility for $U = \infty$ and $\beta = 30$ as a function of δ.

(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 considering 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 have not found any hint of a

ferromagnetic instability at low temperatures close to half-filling. This is consistent with the conjecture that for bipartite lattices—like the simple hypercubic lattice studied here—the critical hole density for the Nagaoka state should be $\delta_c = 0$ [31].

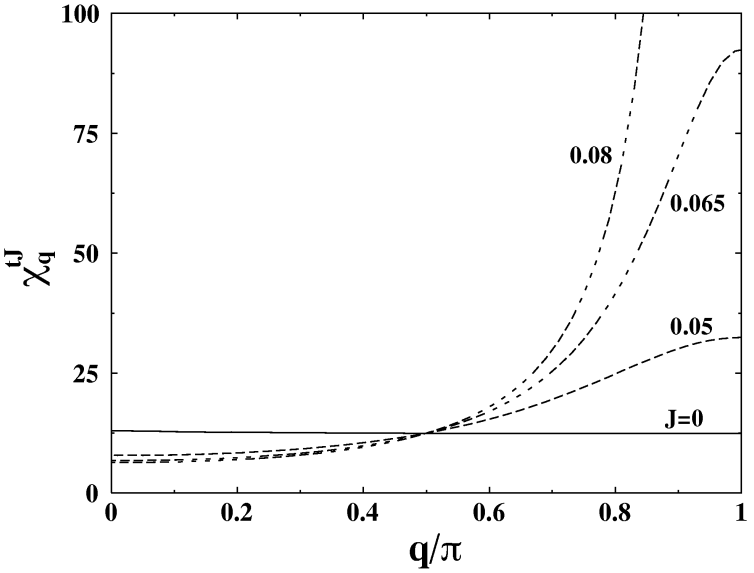

Figure 4. The susceptibility of the t–J model as a function of $\boldsymbol{q}$ for various values of J at a doping $\delta = 5\%$ and for $\beta = 30$.

3.3. Results for the t–J model

Inserting the results for the susceptibility of the HM at $U = \infty$ into equation (9) we obtain the susceptibility for the t–J model as a function of q and J^* as shown in figure 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 dependences of $1/\chi_{AF}^{t-J}$ for a specific value of $J^* = 0.067$ and three dopings $\delta = 2\%$, $\delta = 9\%$ and $\delta = 15\%$ are shown in figure 5. The full curve shows for comparison the case where $\delta = 0$, where one has exactly $1/\chi_{AF}^{t-J} = 2(T - J^*/2)$. As expected for a mean-field theory, close to the antiferromagnetic transition one finds a behaviour $1/\chi_{AF}^{t-J} = (T - T_N)/C_{eff}$ in all cases with decreasing Néel temperature T_N and decreasing effective Curie constant C_{eff} for increasing δ (see, e.g., the inset to figure 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_{eff} vary roughly linearly up to 15% doping. We would also like to point out that 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 $\delta \leqslant 15\%$ and $J^* < 0.12$ are shown in figure 6. One observes the expected increase in the Néel temperature T_N with increasing J^* and a—for larger δ roughly linear—decrease as a function of δ. We may use this approximate linearity of $T_N(\delta)$ to extrapolate the curves $T_N(\delta)$ for a given J^* to $T = 0$.

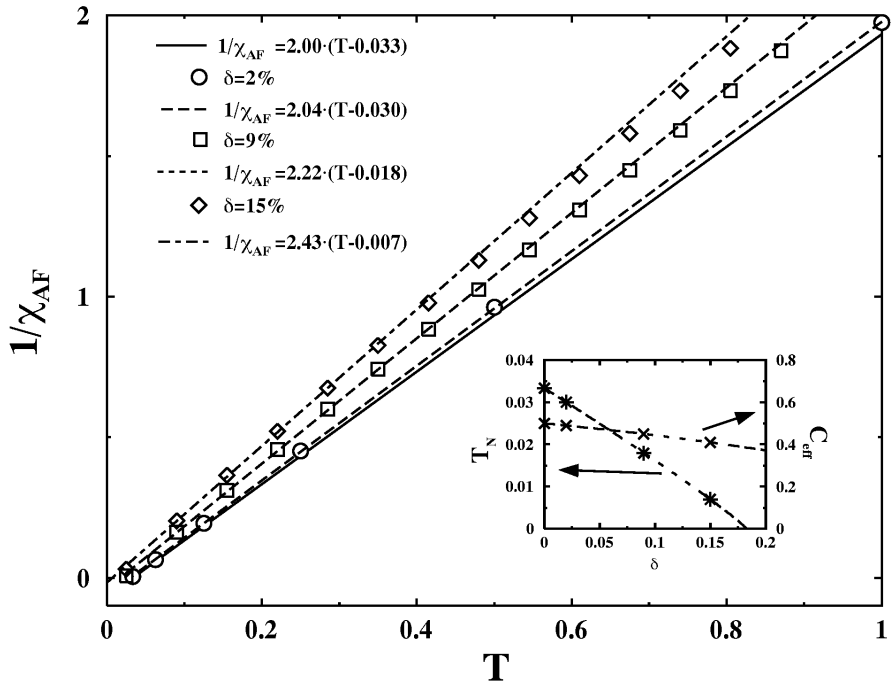

Figure 5. The inverse susceptibility of the t–J model as a function of T for $J^* = 0.067$ and three dopings $\delta = 2\%$, $\delta = 9\%$ and $\delta = 15\%$. Close to the phase transition one observes $\chi_{AF}^{-1}(T) = (T - T_N)/C_{eff}$ as expected for a mean-field theory. Note that for $\delta \to 0$ the linear behaviour is observed up to $T = 1t^*$. The full line represents half-filling, where $\chi_{AF}^{-1} = 2(T - J^*/2)$. The inset shows the dependence of the Néel temperature T_N and effective Curie constant C_{eff} on δ.

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 figure 6. We find that the behaviour of $J_c^*(\delta)$ is rather accurately described by $J_c^* \sim \delta^2$. The phase diagram in figure 6 should be compared to the DMFT results for the Hubbard model in the strong-coupling limit [32]. In [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 δ for large values of U. However, although the value of T_N for $\delta \to 0$ and the observed linearity agree quite well with our results, the decrease of T_N as a function of δ for the Hubbard model at $U = 7t^*$ is much faster than in our figure 6. 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 and J^*, respectively, the Hubbard model and the t–J model are expected to show different physical behaviours: 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 of J^* [5] and may give rise to quite important corrections to physical quantities [33].

Finally we should like to use the observation that close to half-filling the susceptibility

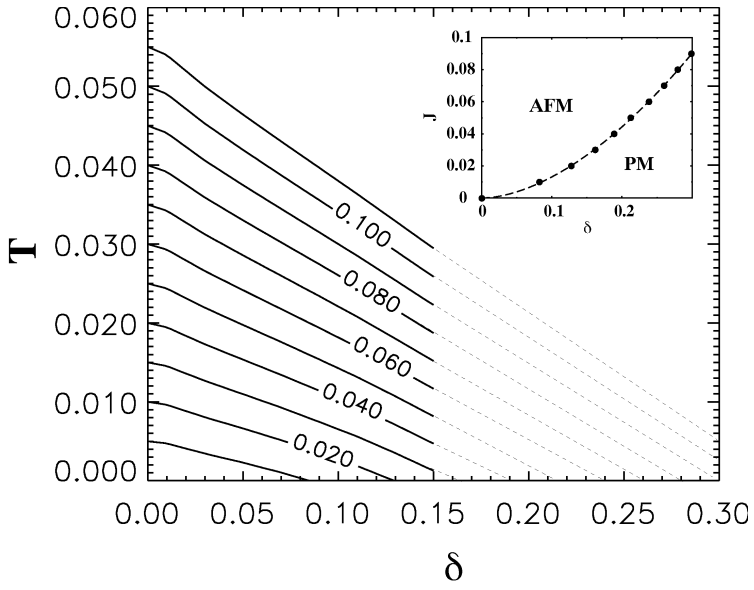

Figure 6. The phase diagram $T_N(\delta, J)$ for the t–J model. The dashed lines represent (linear) extrapolations of the phase boundaries to $T = 0$. The corresponding values of $J_c(\delta)$ behave like $J_c(\delta) \sim \delta^2$, as shown in the inset.

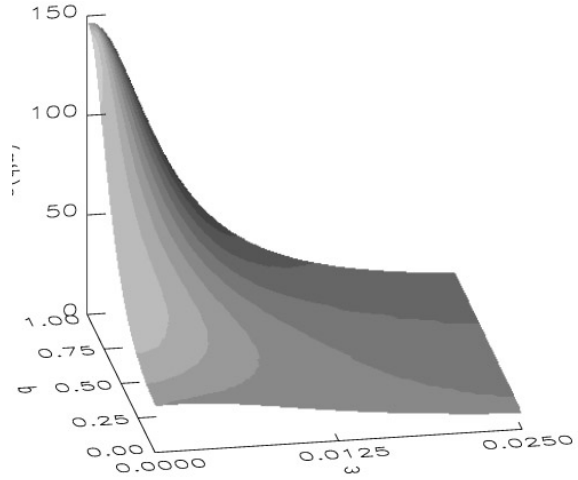

Figure 7. The approximate result for $S_q^{t-J}(\omega)$ for $\delta = 5\%$, $T = 1/30$ and $J = 0.035$.

for the HM is relatively flat with respect to $\boldsymbol{q}$ and obtain an approximation for the dynamical spin structure factor $S(\boldsymbol{q}, \omega) = \mathrm{Im}\, m\chi_{\boldsymbol{q}}(\omega)/(1 - \mathrm{e}^{-\beta\omega})$ by assuming $\chi_{\boldsymbol{q}}^{HM}(\omega) \approx \chi_{loc}^{HM}(\omega)$ in equation (9). This approximation avoids the cumbersome calculation of the $\boldsymbol{q}$-dependent susceptibility for finite frequencies. As an example, the result for $J^* = 0.035$, $T = 1/30$ and $\delta = 5\%$ is shown in figure 7. As expected, the maximum in $S_q^{t-J}(\omega)$ is found at $q = \pi$ and $\omega = 0$ and the intensity decays very quickly with increasing energy for all $\boldsymbol{q}$. 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 have 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, in particular, 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 in terms of the susceptibility of the Hubbard model at $U = \infty$ (cf. equation (9)). In addition the latter can be split into a local part plus a $\boldsymbol{q}$-dependent renormalization which for low doping turned out to be relatively small and only moderately varying with $\boldsymbol{q}$. We find that in the case where $J^* = 0$ (i.e. $U = \infty$) the absence of an explicit magnetic exchange leads to $\chi^{HM}_{q=\pi} \approx \chi^{HM}_{loc}$ 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 susceptibilty at $q = \pi$ and a suppression at $q = 0$ instead. However, for the situation considered here—a 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 the 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 on $\chi^{HM}_{AF}(T, \delta)$ we extracted the phase diagram $T_N(\delta, J^*)$. We found that T_N increases monotonically as a function of J^* and—for fixed J^*—decreases monotonically as a function of δ. For larger doping δ 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 of $T_N(\delta)$ for small U to an almost linear variation for $U \geqslant 7t^*$. However, in contrast to our results one observes a much faster depression of T_N as a function of δ and in addition a transition into an incommensurate phase for large δ. In particular, 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 $\boldsymbol{q}$ was used to set up an approximation for the dynamical susceptibility by assuming $\chi^{HM}_{\boldsymbol{q}}(\omega) \approx \chi^{HM}_{loc}(\omega)$, thus giving to some extent a microscopic justification of the results in [29]. Since in addition $\chi^{HM}_{loc}(\omega)$ can be calculated fairly easy from the effective single-site problem we were able to present results for the dynamical spin structure factor $S^{t-J}_{\boldsymbol{q}}(\omega)$. The general expected features, i.e. a sharp maximum at $q = \pi$ and $\omega = 0$, a shift of the maximum to finite ω for $q < \pi$ and a fast decay for $\omega > 0$, are well reproduced. There are of course several questions left. First of all one should check the assumption of a nearly $\boldsymbol{q}$-independent $\chi^{HM}_{\boldsymbol{q}}(\omega)$ carefully for several values of doping and temperature. Second a systematic study

of $S_q^{t-J}(\omega)$ as a 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 these lines 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 for $d = 2$ or $d = 3$ is unclear. From high-temperature expansions or exact diagonalizations for $d = 2$ one knows, for example, that the static homogeneous susceptibility shows a nonmonotonic behaviour as a function of δ, which may be attributed to fluctuations induced by the spin-flip term in the model (1). Since the DMFT neglects this type of process it is not too surprising that in our results we always observe a monotonic decrease instead. We thus expect that the predictions of the DMFT will be modified not only quantitatively but most likely also qualitatively, especially for two-dimensional systems.

Acknowledgments

We would 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 Forschungsgemeinschaft, grant number Pr 298/3-1.

One of us (TP) also wishes to acknowledge the hospitality of the Department of Physics at the University of Cincinnati, where part of this work was done.

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