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Quasiparticle properties of strongly correlated electron systems with itinerant metamagnetic behavior

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Abstract. A brief account of the zero temperature magnetic response of a system of strongly correlated electrons in strong magnetic field is given in terms of its quasiparticle properties. The scenario is based on the paramagnetic phase of the half-filled Hubbard model, and the calculations are carried out with the dynamical mean field theory (DMFT) together with the numerical renormalization group (NRG). As well known, in a certain parameter regime one finds a magnetic susceptibility which increases with the field strength. Here, we analyze this metamagnetic response based on Fermi liquid parameters, which can be calculated within the DMFT-NRG procedure. The results indicate that the metamagnetic response can be driven by field-induced effective mass enhancement. However, also the contribution due to quasiparticle interactions can play a significant role. We put our results in context with experimental studies of itinerant metamagnetic materials.

PACS. 71.10.Fd Lattice fermion models – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.30.+h Metal-insulator transitions and other electronic transitions – 75.20.-g Diamagnetism, paramagnetism, and superparamagnetism – 71.10.Ay Fermi-liquid theory and other phenomenological models

1 Introduction

The interplay of strong correlation physics and magnetic behavior in itinerant electronic systems has been a fascinating subject for many years. At low temperature it is often possible to describe the response of such systems in terms of the low energy excitations and quasiparticle properties such as in a Fermi liquid picture. The ratio of the spin susceptibility of the interacting system χ_s and that of the non-interacting system χ_s^0 is then given by the expression

$$\frac{\chi_s}{\chi_s^0} = \frac{m^*/m_0}{1+F_0^a}, \tag{1}$$

where m^*/m_0 is the ratio of effective and bare electronic mass, and F_0^a is the lowest order asymmetric Landau parameter, which accounts for quasiparticle interactions. A special kind of response is metamagnetism, which we define here as the existence of a regime where the system's differential susceptibility, $\chi_s = dM/dH$, increases with magnetic field H, i.e. $d\chi_s/dH > 0$, for $H \in [H_1, H_2]$ with $H_1 > 0$. The subject of this paper is the analysis of the metamagnetic response in correlated electron systems in terms of the Fermi liquid description (1). For this we calculate the effective mass and the term due to quasiparticle interactions from a microscopic model. This allows us to understand what drives the magnetic response. This can be relevant for the interpretation of experiments for itinerant metamagnets where the magnetic response is measured simultaneously with the field dependence of the specific heat.

In a naive single electron picture itinerant metamagnetism is not intuitive as with increasing polarization the magnetic response usually decreases. For instance, in weakly interacting systems, such as a Hubbard model with small U, with a featureless concave density of states metamagnetic behavior does not occur. RPA based calculations yield a decreasing susceptibility with increasing field as spin fluctuations are suppressed. On the other hand, a convex density of states, i.e. with positive curvature at the Fermi energy, such as in the Wohlfahrt and Rhodes [1] theory, can lead to metamagnetic behavior. This is exploited in a number of works, where the Hubbard model with such convex density of states is analyzed [2,3]. Metamagnetic behavior is shown to also occur in situations where the Fermi energy lies close to a van Hove singularity [4,5], or where a Pomeranchuk Fermi surface deformation instability occurs [6]. It has been shown by calculations based on the Gutzwiller approximation by Vollhardt [7] and Spalek and coworkers [8–10] that for a generic concave density of states metamagnetic behavior is also found in the intermediate coupling regime of the Hubbard model. The metamagnetic scenario is then that of correlated electrons, with a (Mott) localization tendency due to the interaction.

Our calculations are based on the half filled single band Hubbard model which has been used frequently

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to describe itinerant metamagnetism for correlated electrons [2–5,9–12] due to its relative formal simplicity. We employ the dynamical mean field theory (DMFT) [11,13] combined with the numerical renormalization group (NRG) [14,15] to solve the effective impurity problem. We focus on the case of zero temperature, where sharp features are most clearly visible. We follow these earlier approaches here and restrict ourselves to the response of the paramagnetic solutions of the Hubbard model, which is possible for mean field-like approaches.

The half filled Hubbard model in a magnetic field has already been investigated by detailed DMFT studies by Laloux et al. [11] and Bauer and Hewson [16]. Low temperature magnetization curves and field induced metal insulator transitions have been investigated by Laloux et al. Metamagnetic response based on correlated electron physics, seen in the Gutzwiller approach, was confirmed in such calculations. Our analysis extends previous work [11] as we investigate the $T = 0$ magnetic response with a Fermi liquid interpretation based on the field dependent renormalized parameter approach [16–19]. This, together with results for the spectral functions, allows us to identify what gives rise to the magnetic response in the system.

The paper is organized as follows. In a brief Section 2 we give details about the model and method. The Fermi liquid interpretation and the relation between Fermi liquid parameters and the field dependent renormalized parameters are described in Section 3. Section 4 reports the results for magnetization, susceptibilities and the interpretation in terms of effective mass and quasiparticle interactions. We conclude by putting our results in context with itinerant metamagnetism studied experimentally.

2 Model and method

The basis for our calculation forms the Hubbard Hamiltonian in a magnetic field, which in the grand canonical formulation reads

$$H_\mu = \sum_{i,j,\sigma} (t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c) - \sum_{i\sigma} \mu_\sigma n_{i\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \tag{2}$$

$c^\dagger_{i,\sigma}$ creates an electron at site i with spin σ, and $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$. $t_{ij} = -t$ for nearest neighbors is the hopping amplitude and U is the on-site interaction; $\mu_\sigma = \mu + \sigma h$, where μ is the chemical potential of the interacting system, and the Zeeman splitting term with external magnetic field H is given by $h = g\mu_B H/2$ with the Bohr magneton μ_B. In the DMFT approach the proper self-energy is a function of ω only [20,21]. In this case the local lattice Green's function $G^{\rm loc}_\sigma(\omega)$ can be expressed in the form,

$$G^{\rm loc}_\sigma(\omega) = \int d\varepsilon \, \frac{\rho_0(\varepsilon)}{\omega + \mu_\sigma - \Sigma_\sigma(\omega) - \varepsilon}, \tag{3}$$

where $\rho_0(\varepsilon)$ is the density of states for the non-interacting model ($U = 0$). It is possible to convert this lattice problem into an effective impurity one [13], introduce the dynamical Weiss field $\mathcal{G}^{-1}_{0,\sigma}(\omega)$. The DMFT self-consistency condition reads

$$\mathcal{G}^{-1}_{0,\sigma}(\omega) = G^{\rm loc}_\sigma(\omega)^{-1} + \Sigma_\sigma(\omega). \tag{4}$$

The Green's function $G^{\rm loc}_\sigma(\omega)$ can be identified with the Green's function $G_\sigma(\omega)$ of an effective Anderson model, and $\mathcal{G}^{-1}_{0,\sigma}(\omega)$ expressed as

$$\mathcal{G}^{-1}_{0,\sigma}(\omega) = \omega + \mu_\sigma - K_\sigma(\omega). \tag{5}$$

The function $K_\sigma(\omega)$ plays the role of a dynamical mean field describing the effective medium surrounding the impurity. $K_\sigma(\omega)$ and $\Sigma_\sigma(\omega)$ have to be calculated self-consistently using equations (3)–(5). Our calculations are based on the numerical NRG [14,15] to solve the effective impurity problem. As in earlier work [16] we calculate spectral functions from a complete basis set [22,23] and use higher Green's functions to obtain the self-energy [24]. For numerical calculations within the DMFT-NRG approach for $\rho_0(\varepsilon)$ we take the semi-elliptical form for the non-interacting density of states $\rho^{\rm sem}_0(\varepsilon) = 2\sqrt{D^2 - \varepsilon^2}/\pi D^2$, where $W = 2D$ is the band width with $D = 2t$ for the Hubbard model. $t = 1$ sets the energy scale in the following.

3 Field dependent renormalized parameters and Fermi liquid theory

The response of a metallic system of correlated electrons can often be described in terms of Fermi liquid theory. The ratio of the spin susceptibility of the interacting system χ_s and that of the non-interacting system χ^0_s is given in equation (1). Thus, when strongly interacting fermions have a large paramagnetic susceptibility, it can be interpreted as due to quasiparticles with large effective masses. It is, however, also possible that the susceptibility is additionally enhanced due to the quasiparticle interaction term $1/[1 + F^a_0]$, which is for instance the case in liquid ^{3}He, where $m^*/m_0 \simeq 5$ but $\chi_s/\chi^0_s \simeq 20$ [25]. This is usually described by the dimensionless Sommerfeld or Wilson ratio R of the magnetic susceptibility and the linear specific heat coefficient γ. We will use it in the form $R = (\chi_s/\chi^0_s)/(\gamma/\gamma_0)$, where $\gamma/\gamma_0 = m^*/m_0$.

Here we are interested in analyzing the behavior in finite field, and it is possible to calculate corrections of higher order in H to equation (1) [26]. We will, however, follow a different approach here, and assume that expression (1) remains valid for finite field with field dependent effective mass $m^*(H)$ and Landau parameter $F^a_0(H)$. This is in the spirit of the field dependent quasiparticle parameters introduced in earlier work [16,18,19]. Notice that for the case considered the field dependence of χ^0_s, which is given by the non-interacting density of states, varies very little in the relevant field range. In this picture with field dependent parameters, metamagnetism can occur when the effective mass increases with the magnetic field. Generally, however, also the field dependence of the quasiparticle interaction plays a role. One hypothesis tested in this

paper is that itinerant metamagnetic behavior is always accompanied by a field induced localization and a sharp increase of the effective mass near the metamagnetic transition.

In order to calculate the microscopic Fermi liquid parameters, we expand $\Sigma_\sigma(\omega)$ in powers of ω for small ω, and retain terms to first order in ω only. This is used to define renormalized parameters [16],

$$\tilde{\mu}_{0,\sigma} = z_\sigma[\mu_\sigma - \Sigma_\sigma(0)], \quad \text{and} \quad z_\sigma = 1/\left[1 - \Sigma'_\sigma(0)\right], \quad (6)$$

and from (3) a normalized quasiparticle propagator,

$$\tilde{G}^{\rm loc}_{0,\sigma}(\omega) = \frac{1}{z_\sigma}\int d\varepsilon\, \frac{\rho_0(\varepsilon/z_\sigma)}{\omega + \tilde{\mu}_{0,\sigma} - \varepsilon}. \quad (7)$$

Note that this ω-expansion can also be carried out in finite magnetic field. Then the renormalized parameters become field dependent, $z_\sigma = z_\sigma(h)$ and $\tilde{\mu}_{0,\sigma} = \tilde{\mu}_{0,\sigma}(h)$. The density of states $\tilde{\rho}_{0,\sigma}(\varepsilon)$ derived from (7), $\tilde{\rho}_{0,\sigma}(\varepsilon) = -{\rm Im}\tilde{G}_{0,\sigma}(\varepsilon + i\delta)/\pi = \rho_0[(\varepsilon + \tilde{\mu}_{0,\sigma})/z_\sigma]/z_\sigma$, is referred to as the free quasiparticle density of states. z_σ is interpreted as the weight of the quasiparticle resonance and $\tilde{\mu}_{0,\sigma}$ gives the position of the quasiparticle band. All energies are measured from the chemical potential μ.

To obtain the renormalized parameters z_σ and $\tilde{\mu}_{0,\sigma}$, we use two different methods based on the NRG approach. The first method is a direct one where we use the self-energy $\Sigma_\sigma(\omega)$ determined by NRG and the chemical potential μ_σ, and then substitute into equation (6) for z_σ and $\tilde{\mu}_{0,\sigma}$. The second method is indirect, and it is based on the quasiparticle interpretation of the NRG low energy fixed point of the effective impurity [17]. This approach has been used earlier for the Hubbard model [16,27] and for the Anderson impurity model in a magnetic field [18,19]. As shown before the results of both methods usually agree within a few percent, and we use an average value of both methods for the numerical results. It is important to calculate these parameters accurately, since for the following results also their derivatives are needed.

We can calculate static expectation values and response functions in terms of the renormalized parameters. The quasiparticle occupation number $\tilde{n}^0_\sigma$ is given by integrating the quasiparticle density of states up to the Fermi level,

$$\tilde{n}^0_\sigma = \int_{-\infty}^{0} d\varepsilon\, \tilde{\rho}_{0,\sigma}(\varepsilon) = \int_{-\infty}^{\infty} d\varepsilon\, \rho_{0,\sigma}(\varepsilon)\theta(\mu_\sigma - \Sigma_\sigma - \varepsilon). \quad (8)$$

Luttinger's theorem [28] holds for each spin component for the Hubbard model in magnetic field [16], hence we have $\tilde{n}^0_\sigma = n_\sigma$, where n_σ is the value of the occupation number in the interacting system at $T = 0$.

To calculate the magnetic response we focus for the rest of this paper on the case with particle-hole symmetry where $\mu = U/2$, and we can write $\Sigma_\sigma(0,h) = U/2 - \sigma\eta(h)$. We can calculate $\eta(h)$ directly from the self-energy, e.g. $\eta(h) = (\Sigma_\downarrow - \Sigma_\uparrow)/2$, or from the renormalized parameters $\eta(h) = \tilde{\mu}_0(h)/z(h) - h$. At half filling we have $z_\uparrow = z_\downarrow \equiv z$ and $\tilde{\mu}_{0,\uparrow} = -\tilde{\mu}_{0,\downarrow} \equiv \tilde{\mu}_0$. We define the function

$$g(h) := h + \eta(h) = \tilde{\mu}_0(h)/z(h) = \tilde{\mu}_0(h)m^*(h)/m_0, \quad (9)$$

as $m^*/m_0 = z^{-1}$ in DMFT. In terms of the quasiparticles it is the product of the effective mass enhancement m^*/m_0 and the shift of the quasiparticle band $\tilde{\mu}_0$. With the applicability of Luttinger's theorem the magnetization is then given by

$$m(h) = \frac{1}{2}(n_\uparrow - n_\downarrow) = \int_{-\infty}^{\infty} d\varepsilon\, \rho_0(\varepsilon)\theta[g(h) - \varepsilon] - \frac{1}{2}. \quad (10)$$

For a local self-energy this is an exact expression for the magnetization, which only depends on the field dependent renormalized parameters via $g(h)$. For certain bare densities of state, for instance, for the semi-elliptical density of states $\rho_0^{\rm sem}(\varepsilon)$, it can be evaluated analytically,

$$m(h) = \frac{1}{2}g(h)\rho_0^{\rm sem}(g(h)) + \frac{1}{\pi}\arcsin(g(h)). \quad (11)$$

Differentiating (10) with respect to h yields the local static spin susceptibility

$$\chi_s = \frac{dm}{dh} = g'(h)\rho_0(g(h)) \quad (12)$$

where here and in the following primes indicate derivatives with respect to h. A similar expression had already been derived by Luttinger [28]. The metamagnetic condition $\chi'_s(h) > 0$ is then

$$g''(h)\rho_0(g(h)) + \rho'_0(g(h))g'(h)^2 > 0. \quad (13)$$

The occurrence of metamagnetic behavior can be analyzed depending on the functional form of $g(h)$ and $\rho_0(\varepsilon)$. For a simple analysis let us assume $h > 0$ and the power law form for $g(h) = c\,h^\alpha$, $c > 0$. The first term in (13) is then positive if $\alpha > 1$. For a convex density of states, $\rho''_0(\varepsilon) > 0$, the second term is also positive and metamagnetic behavior occurs as mentioned earlier. For a concave density of states, $\rho''_0(\varepsilon) < 0$, the two terms in (13) compete. If we also assume the power law form for the density of states, $\rho_0(\varepsilon) = r_0 - d\,\varepsilon^\gamma$, (e.g. for $\rho_0^{\rm sem}$ one has $r_0 = 2/\pi D$ $d = r_0/2$ and $\gamma = 2$) condition (13) becomes

$$\frac{r_0}{c^\gamma d}\frac{\alpha - 1}{\alpha(1+\gamma) - 1} > h^{\alpha\gamma}. \quad (14)$$

Since the right hand side is positive, we can infer that for $\alpha > 1$ and $\gamma > (1-\alpha)/\alpha$ metamagnetic behavior occurs. The actual field dependence of $g(h)$ can be calculated from the renormalized parameters and it depends on the interaction strength. As we will see for the half filled Hubbard model and intermediate U, $g(h)$ grows faster than linear with h, i.e. $\alpha > 1$.

In the limit of zero field the ratio of the susceptibility of the interacting and non-interacting system has a simplified expression in terms of the renormalized parameters,

$$\frac{\chi_s}{\chi_s^0} = g'(0) = \frac{m^*(0)}{m_0}\tilde{\mu}'_0(0), \quad (15)$$

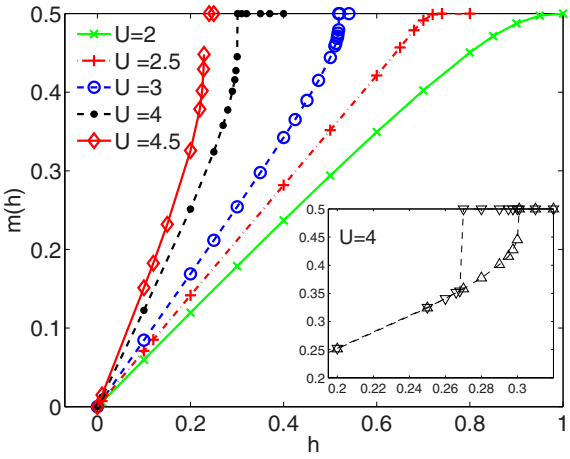

Fig. 1. (Color online) The local magnetization $m(h)$ as a function of the magnetic field h for different values of U. We can see that a metamagnetic curvature sets in at $U = 3$. Inset: Hysteresis curve for $U = 4$ (triangle up increasing h, triangle down decreasing h).

for $\tilde{\mu}_0(0) = 0$. Comparing with the Fermi liquid expression (1) we can identify $1/(1 + F_0^a) = \tilde{\mu}_0'$. This quantity corresponds to the Wilson ratio R. In the general case, the field dependent enhancement due to the quasiparticle interactions reads

$$R(h) = \frac{1}{1 + F_0^a(h)} = \left(\tilde{\mu}_0' + \tilde{\mu}_0 \frac{m^{*\prime}}{m^*}\right) \frac{\rho_0\left(\tilde{\mu}_0 \frac{m^*}{m_0}\right)}{\rho_0(h)}. \quad (16)$$

So far the considerations have been independent of our DMFT-NRG approach. In the following section we will compare results for the magnetic susceptibility obtained from the static expectation values of integrating the Green's functions, with the results based on the field dependent parameters. We determine them as described above. Alternatively they can be calculated by other methods, such as the Gutzwiller (GW) approach, and we will make comparison as appropriate. Results are obtained as in reference [7], where the critical interaction for the metal insulator transition is $U_c^{\mathrm{GW}} = 16W/3\pi \approx 6.79$ for $\rho_0^{\mathrm{sem}}(\varepsilon)$ with $W = 4$.

4 Results

4.1 Magnetization and metamagnetic transition

For a first overview we present results for the magnetization $m(h)$ as a function of field h in Figure 1 for various values of U. The magnetization $m(h)$ was computed from the static NRG expectation value (EV) for the occupation number as well as from integrating the spectral function to the Fermi level, both of which agree very well. The results for $m(h)$ based on the field dependent renormalized parameters (RP) and equation (11) are also in good agreement, but not included in the figure.

The plot gives a clear picture of the field strength h_{pol} necessary to polarize the metal completely to $m = 1/2$. For weak coupling it can be related to the rigid band shift and a large field $h \sim D$ is needed, but for larger interaction strength h_{pol} is reduced substantially. For $U \geq 3$ a metamagnetic curvature in the magnetization can be observed, and we see that in the Hubbard model at zero temperature the metamagnetic transition field[1] h_{m} coincides with h_{pol}, which is not necessarily the case for $T > 0$. Laloux et al. [11] have compared results from low temperature DMFT calculations with the Gutzwiller approximation and it was found that the occurrence of metamagnetic behavior is overestimated by the Gutzwiller approximation (see also Fig. 3).

Earlier work [11] showed that the transition is a discontinuous first order one at low temperature. Our results show jumps in the magnetization curve at the transition field h_{m}, e.g. for $U = 3$ and $U = 4$ in Figure 1, however, we can not exclude a very steep continuous increase which can not be resolved numerically. We have also found hysteresis, shown for $U = 4$ as an inset in Figure 1 (triangle up increasing h, triangle down decreasing h). This suggests that the transition is also of first order for zero temperature. For larger interaction $U \geq 4.5$ there exists a small field range near h_{m}, where we have not found unique, well converged DMFT solutions, so no definite statement can be made.

The half filled repulsive Hubbard model in magnetic field can be mapped to the attractive one [29], in which the chemical potential is related to the field in the original model, $\mu = U/2+h$. The attractive model has been studied by the DMFT in situations, where superconducting order was not allowed for [30,31]. A first order transition from a metallic to a pairing state for fixed density was found at a critical interaction. The occurrence of the transition can be related to the metamagnetic transition here. A nearly polarized system corresponds to a low density limit, and to estimate when the transition sets in, one can analyze the two-body problem in the attractive model and calculate the critical U_c for bound state formation. For a three dimensional cubic lattice the result is $U_c \approx 0.659W$ [29]. With the given bandwidth this corresponds to a value of $U_c \approx 2.64$, which is a reasonable estimate for the interaction strengths, where the metamagnetic behavior is found here.

4.2 Magnetic susceptibilities and quasiparticle properties

From the initial slope of the magnetization curves in Figure 1 we observe an increase of the magnetic susceptibility with the interaction strength U. This increase can also be seen in the following Figure 2 where we show the ratio of zero field susceptibility to the non-interacting value χ_s^0 as function of U deduced from differentiating the EV for $m(h)$ in the limit $h \to 0$.

For comparison we have also included the susceptibility calculated from equation (15) with the renormalized

[1] The metamagnetic transition field is the field where the susceptibility is maximal.

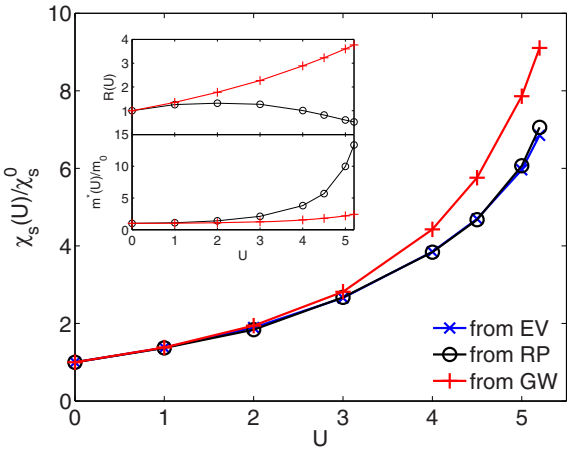

Fig. 2. (Color online) The U-dependence of the magnetic susceptibility χ_s. We compare results deduced from the EV of $m(h)$ with ones obtained from the RP and from the Gutzwiller (GW) approximation. The inset shows the effective mass $m^*(U)/m_0$ and the Wilson ratio $R(U)$ as a function of U.

parameters (RP) and their derivatives, as well as the results obtained from the Gutzwiller (GW) approximation. EV and RP results agree very well, confirming the applicability of Fermi liquid results in this metallic regime. The GW results follow a similar trend but overestimate the value for the susceptibility, which becomes more pronounced for larger U.

The inset plot shows the U-dependence of the effective mass and the Wilson ratio. In terms of Fermi liquid theory and the expression (1) the increase of χ_s with U can be understood by the behavior of the effective mass and the progressive localization tendency, which brings out more the spin degrees of freedom of the electrons. We can see, however, that the effective mass ratio is larger than that of the magnetic susceptibility. This difference can be attributed to the factor $R = \tilde{\mu}_0' = [1+F_0^a]^{-1}$, which is due to the quasiparticle interaction. This factor is larger than one for smaller values of U, but decreases to values below one for stronger interaction. This indicates a sign change of the parameter F_0^a from negative to positive. The comparison with the corresponding quantities calculated in the GW approximation shows a qualitatively similar behavior for both m^*/m_0 and R, when U is small. For larger values of U in Figure 2, however, the effective mass enhancement in the GW approach, $m^*/m_0 = 1 - (U/U_c^{\rm GW})^2$, is much smaller and R increases with U in contrast to the DMFT result.

We return to the finite field response and focus on the metamagnetic behavior which is found for intermediate values of U. Results for the ratio of the magnetic susceptibility in finite and zero field deduced from differentiating the magnetization (EV) are compared to the ones obtained from the quasiparticle parameters (RP) and equation (12). For completeness, we have also included results from the GW approximation. This is shown in Figure 3 for $U = 3$ in the upper panel and $U = 4.5$ in the lower panel.

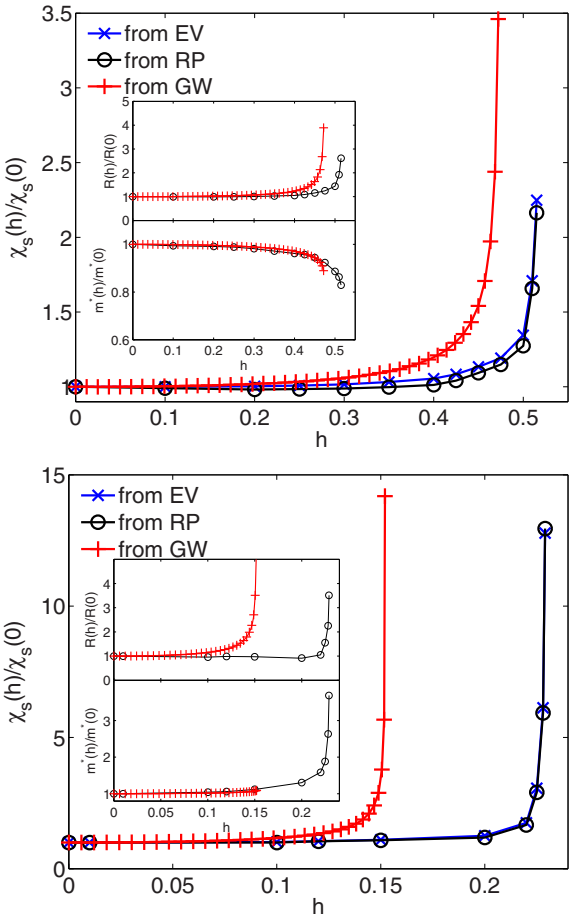

Fig. 3. (Color online) The h-dependence of the ratio of the finite and zero field magnetic susceptibility χ_s for $U = 3$ (upper panel) and $U = 4.5$ (lower panel). We compare results deduced from the EV for $m(h)$ with ones obtained from the RP and the ones from the GW approach. The inset shows the ratio of finite and zero field effective mass $m^*(h)/m_0(0)$ and the Wilson ratio $R(h)/R(0)$ as a function of h.

We can see that also in finite field the results for the susceptibility calculated from the EV for $m(h)$ and the field dependent RP agree fairly well with a deviation of less than 5%. For the case $U = 3$ (upper panel) the results for $\chi(h)$ based on the field dependent RP are always smaller. In both cases we find first a period where the susceptibility is nearly constant, but then starts to increase rapidly as h approaches $h_{\rm m}$. For $U = 3$ the values obtained from the RP initially decrease slightly with the field, which is however incorrect, and comes about through numerical inaccuracies when determining the parameters and the numerical differentiation. As $h_{\rm m} = h_{\rm pol}$ the magnetic susceptibility is zero for $h > h_{\rm m}$. At finite temperature a susceptibility maximum is expected. The results for χ_s from the GW approximation show generally a similar trend, but as mentioned earlier the metamagnetic behavior sets in at lower field strengths.

A difference in the behavior between the two cases is visible in the two insets where the ratios of field dependent effective masses to their zero field values and the

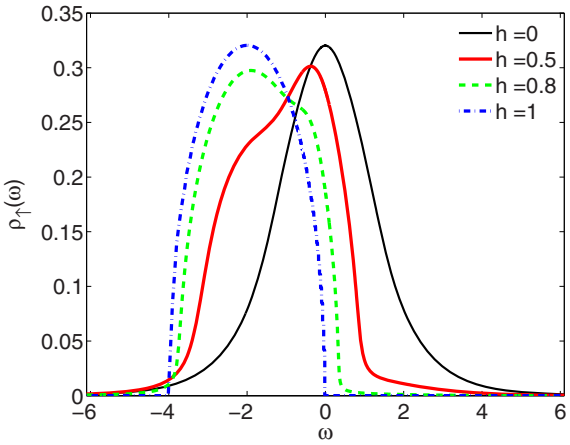

Fig. 4. (Color online) The majority spin density of states for $U = 2$ and various field strengths in comparison.

field dependent Wilson ratios $R(h)/R(0)$ are plotted. For the $U = 3$ case the effective mass decreases with the field which is typical behavior in the weak coupling regime. It can be understood by RPA approximations where spin fluctuations, which give an effective mass enhancement, are suppressed in finite field. The metamagnetic increase of the susceptibility, however, can not be explained by this. In terms of Fermi liquid theory it is related to the magnetic field dependence of the quasiparticle interaction rather than the localization tendency encoded in the effective mass. $R(h)/R(0)$ indeed is increasing sharply close to $h_{\rm m}$. In equation (16) we have two competing terms for this enhancement factor, $m^{*\prime}/m^* < 0$, but one finds $\tilde{\mu}_0' > |\tilde{\mu}_0\, m^{*\prime}/m^*|$ which leads to the observed enhancement. The drive for the metamagnetic behavior is therefore due to the shift of the quasiparticle band from the Fermi level with increasing field. This contrasts to the weak coupling situation, such as $U = 2$, where $R(h)$ decreases with the field strength and no metamagnetic response is observed.

The effective mass in the case of $U = 4.5$ (lower panel in Fig. 3) shows different behavior. We can see a sharp increase with the field. However, the magnitude the ratio m^*/m_0 increases is less than that of the susceptibility. The difference again can be related to the Fermi liquid factor $R = 1/[1 + F_0^a]$, which is larger than one and increasing with h as can be seen in the inset of the lower panel in Figure 3. In this case the second term in equation (16) is positive and the first term negative, but $|\tilde{\mu}_0'| < |\tilde{\mu}_0\, m^{*\prime}/m^*|$. The results from the GW approach for the effective mass and R are in line with the DMFT calculations for the case $U = 3$, however, for $U = 4.5$, the GW result for $m^{*\prime}/m^*$ only increases very little with the field, whereas $R(h)$ increases sharply to yield the metamagnetic response.

For larger interactions than the ones discussed here ($5 < U < U_c$), one can encounter difficulties to reach convergency in the DMFT calculations with finite field as discussed in earlier work [16]. The results indicate, however, that there is a strong field dependent enhancement of the effective mass which is the main drive for the metamagnetic response. The ratio $R(h)/R(0)$ varies little with

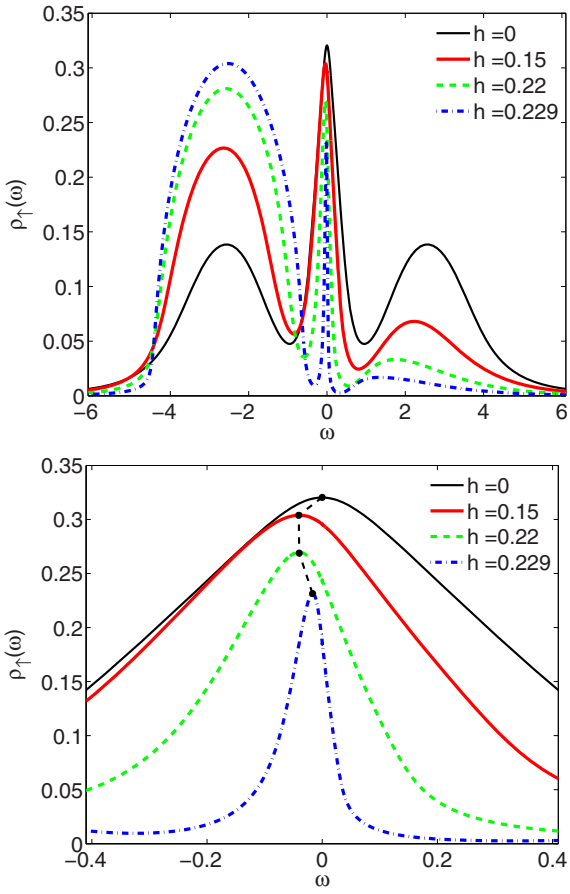

Fig. 5. (Color online) The majority spin density of states for $U = 4.5$ and various field strengths in comparison: upper panel full frequency range, lower panel low frequency behavior.

h or even decrease for larger fields. Such a behavior is also found within the GW approach for larger U near the metal insulator transition.

4.3 Spectral functions

The behavior of the quasiparticle band can be seen directly in the local spectral function. For the cases with smaller coupling the field dependent response shows a continuous shift of spectral weight to lower energies for the majority spin (see Fig. 4 for $U = 2$).

Note that the minority spin density of states $\rho_\downarrow(\omega)$ is given by $\rho_\uparrow(-\omega)$ at half filling. To illustrate the behavior of the quasiparticle peak for the stronger interacting case with $U = 4.5$ in more detail, we plot the local spectral function for the majority spin $\rho_\uparrow(\omega)$ in Figure 5.

In the upper panel we can see how the lower Hubbard peak in the spectral density acquires weight when the field and thence magnetization is increased whilst the upper Hubbard peak loses spectral weight. The behavior at low energy is seen more clearly in the lower panel. At first sight the overall picture is reminiscent of the particle hole symmetric Anderson impurity model in the Kondo regime in magnetic field [18] as far as the high energy behavior is

concerned. The quasiparticle resonance in the locally correlated system broadens and departs from the Fermi level. This behavior occurs in an analogous fashion in the weak coupling regime of the Hubbard model with $\tilde{\mu}_0'(h) > 0$. In the strongly correlated case, however, we find a significant narrowing of the quasiparticle peak in the field, which is accompanied by the field induced metal insulator transition and metamagnetic behavior. The quasiparticle resonance first departs from the Fermi energy, but for larger fields is driven back to it. These features are visible in the field dependence of the renormalized parameter $\tilde{\mu}_0$ with $\tilde{\mu}_0' < 0$ as discussed above.

5 Relation to experiments and conclusions

It is of interest to see, whether the described behavior bears any resemblance with what is observed experimentally in strongly correlated itinerant electron system. Metamagnetic behavior is observed, for instance, in the heavy fermion compounds $CeRu_2Si_2$ [32,33], UPt_3 [34] or $Sr_3Ru_2O_7$ [33,35–37] and the Co-based metallic compounds such as $Y(Co_{1-x}Al_x)_2$ [38,39], sometimes called nearly ferromagnetic metals. The microscopic origin for the occurrence of the effect in these compounds can be manifold, and is sometimes still controversial. In many cases antiferromagnetic exchange is thought be important and the system's closeness to a magnetic instability.

For generic features, we attempt to compare our microscopic Fermi liquid description with experimental studies of itinerant metamagnetic behavior in heavy fermion compounds. It is important, however, to be aware that our results based on the paramagnetic solutions of the half filled single band Hubbard model are not appropriate to make quantitative predictions for those complex systems. Organic conductors are thought to behave like simple Mott-Hubbard systems and have been shown to display a magnetic field induced localization transition with hysteresis by resistance measurements [40]. The author is, however, not aware of any published field dependent magnetization or specific heat data to compare to.

In materials such as $CeRu_2Si_2$, UPt_3 or $Sr_3Ru_2O_7$ the magnetic field dependence of the linear specific heat coefficient γ was measured near the metamagnetic transition [32–34,37]. It is worth noting that, as can be shown from a thermodynamic identity, the field dependence of γ can also be extracted from T^2-coefficient of the magnetization [32]. In the experiments γ increases with the magnetic field and possesses a maximum at the metamagnetic transition $h = h_m$. This is comparable with the Fermi liquid results for stronger coupling, e.g. the case $U = 4.5$ (Fig. 3 lower panel), where the effective mass increases with the magnetic field. In the case of $CeRu_2Si_2$ [33] one can see that the susceptibility increase with the magnetic field is up to about 8.5 times the zero field value, whereas in the same regime the specific heat coefficient only shows an enhancement of 1.6. In our Fermi liquid interpretation this signals that the quasiparticle interaction plays an important role in the susceptibility enhancement and the metamagnetic behavior. The relevance of this has been emphasized in the recent experimental work on Yb_3Pt_4 [41]. A more careful quantitative comparison would be possible based on the periodic Anderson model, for instance. The present approach can be extended to this situation, but also other techniques are available [42–45].

To summarize, we have analyzed the metamagnetic response of the half filled Hubbard model in terms of renormalized quasiparticle parameters and Fermi liquid theory. The renormalized parameters can be calculated accurately with methods based on the NRG, and they have a clear physical meaning. It is shown that the field dependent metamagnetic behavior can have part of its origin in field induced effective mass enhancements, but is not fully explained by this. This is most clearly pointed out in Figure 3, where metamagnetic behavior for smaller U is accompanied by an effective mass reduction in the field, whereas for larger interaction the opposite is the case. The comparison with results obtained from the Gutzwiller approximation gives similar trends, but shows quantitative deviations. The hypothesis that the metamagnetic behavior in itinerant systems is always driven by field induced mass enhancement is therefore found to be not valid. In the intermediate coupling regime it is also shown that the effective mass enhancement alone is not sufficient to explain the metamagnetic enhancement and based on Fermi liquid theory arguments the quasiparticle interaction has to account for the difference. As a generic feature there the corresponding term described by the Wilson ratio R increases near the metamagnetic transition. The opposite happens in the weak (no metamagnetic response) and strong coupling situation. The observation that only a part of the susceptibility enhancement is based on the effective mass is found to be qualitatively in agreement with experimental observations in heavy fermion systems.

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