Field-dependent dynamics in the metallic regime of the half-filled Hubbard model

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Abstract
A systematic study of the effect of magnetic field ($h$) on the Hubbard model has been carried out at half-filling within dynamical mean field theory. In agreement with previous studies, we find a zero temperature itinerant metamagnetic transition, reflected in the discontinuous changes in magnetization as well as in the hysteresis, from a paramagnetic (PM) metallic state to a polarized quasi-ferromagnetic (QFM) state, at intermediate and large interaction strengths ($U$). The jump in magnetization vanishes smoothly with decreasing interaction strength, and at a critical $U$, the transition becomes continuous. The region of ‘coexistence’ of the PM and QFM solutions in the field–$U$ plane obtained in this study agrees quantitatively with recent numerical renormalization group calculations, thus providing an important benchmark. We highlight the changes in dynamics and quasiparticle weight across this transition. The effective mass increases sharply as the transition is approached, exhibiting a cusp-like singularity at the critical field, and decreases with field monotonically beyond the transition. We conjecture that the first order metamagnetic transition is a result of the competition between Kondo screening, that tries to quench the local moments, and Zeeman coupling, which induces polarization and hence promotes local moment formation. A comparison of our theoretical results with experiments on $^3$He indicate that a theory of $^3$He based on the half-filled Hubbard model places it in a regime of intermediate interaction strength.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
One of the most interesting aspects of strongly correlated electrons is the self-consistent emergence of a low energy scale [1]. This has been demonstrated over the years from a large number of theoretical and experimental studies. The Kondo quenching of local moments and the emergence of a Fermi liquid below a critical temperature in Mott–Hubbard systems is clearly seen in dynamical mean field theory (DMFT). A question, therefore, naturally arises as to how an external magnetic field would interact with the local moments and how the Mott–Hubbard physics gets affected by this added field that couples with the moments.

The Mott–Hubbard systems like ($V_1-x\text{Cr}_x$)$_2$O$_3$ [2], $V_2O_3$ [3] display local magnetic moments which also interact through residual antiferromagnetic exchange. There is competition between the alignment of the local moments in the presence of a magnetic field and the residual antiferromagnetic exchange. Magnetic transitions are known to occur in the half-filled Hubbard model [4, 5] in the insulating state. Of course, the problem is more involved in the metallic side due to the presence of an additional energy scale (the local Kondo temperature), associated with the quenching of local spin fluctuations at low temperature. So, the question raised above is much more subtle in the metallic phase of the Mott–Hubbard system. A quantitative study of the dynamics and transport properties of this model is not easy. Recently, much progress has been made with the advent of DMFT [6–9] which is exact in the limit of infinite spatial dimension. Within DMFT, a correlated model maps onto a single-impurity model in a self-consistent conduction-electron bath. Methods like the numerical renormalization group (NRG) [10], local moment approach (LMA) [11–13], exact diagonalization (ED) [8], quantum Monte Carlo (QMC) [8] and iterative perturbation...
theory (IPT) [14–16] have been used to study the impurity problem within the DMFT framework. Mott transition has been observed in the half-filled Hubbard model using DMFT [4, 5].

Prior to the advent of DMFT, there were two major approaches for strongly correlated Fermi liquids—the Stoner approach [18–20] and the Gutzwiller approach (GA) [21–23]. The former approach views the system as close to a ferromagnetic transition and the latter views it as a strongly correlated, nearly incompressible Fermi liquid close to a Mott localization. While the Stoner theory is essentially a high temperature approach, the GA starts from a Hubbard model description of the strongly correlated electrons and projects out the local double occupancies from the ground state in a variational calculation. The GA is incapable of describing the metallic phase of the half-filled Hubbard model, and also fails to incorporate any dynamics or temperature dependence. However, it does have the merit of being analytically tractable, and thus can yield qualitative insight, provided the results have been benchmarked against other detailed calculations. These two approaches have very different predictions for the response to an external magnetic field. The Stoner approach predicts a smooth variation of magnetization in the presence of a magnetic field while the GA gives a first order transition of the magnetization. Experimentally, an effort to distinguish between the two predictions, based on studies in liquid $^3$He [24], finds a smooth variation of the magnetization as predicted in the Stoner approach. Within DMFT, calculations [25] using exact diagonalization (ED) as the impurity solver were carried out to study the effect of magnetic field on the Hubbard model. A fictitious temperature scale was introduced through a frequency cutoff. The calculations were carried out at a fixed magnetization. A metamagnetic transition was obtained, and the $T-U$ ‘phase diagram’ was extended to the finite field axis, that demonstrated a similarity between the effects of temperature and field. A qualitative agreement with the GA was also found.

Later, an exchange term was introduced [26] to incorporate the spin–spin correlation to combine features of Mott localization and almost ferromagnetic Stoner instability. Changes in dynamics with applied field, however, were not studied in these papers. A recent study of the same problem was carried out by Bauer [27] using the numerical renormalization group method within DMFT. The focus in this study was on the metamagnetic transition, and the results were qualitatively similar to the earlier work; the main result being that the divergence of susceptibility at the metamagnetic transition is not a consequence of effective mass divergence but occurs through the quasiparticle interaction term. The prediction for the coexistence region in the $h-U$ plane was not made explicitly in the NRG study; nevertheless, it is possible to deduce this from the results presented. There appears to be a strong disagreement between the NRG and ED study in this context.

In this paper, we study the effects of magnetic field on correlated electron liquids within the framework of the half-filled Hubbard model, using the iterated perturbation theory (IPT) as the impurity solver for the DMFT. The relative merits and demerits of the IPT are discussed in the next section. Since DMFT is known to treat the local dynamics quite accurately, it is expected to reveal the local nature of the competition between the spin fluctuation and the aligning field. We calculate the single particle dynamics, magnetization and other properties of the Hubbard model in the presence of an external magnetic field. In the infinite dimensional limit, the magnetic field appears only as a Zeeman term and there is no explicit orbital contribution in the Hamiltonian as the lattice model is mapped onto a single-impurity model. There are no non-local terms, and the effects due to the non-interacting medium are included as a dynamical mean field in the hybridization. Our focus in this study is on the field-induced changes in quasiparticle weight and spectral functions as the interaction strength is varied. Although the DMFT + NRG study by Bauer [27] does examine dynamics, the detailed behaviour of the crossover from the low field Fermi liquid behaviour to the high field non-Fermi liquid behaviour was not examined. Such a crossover was proposed in the DMFT + ED work [25], but was not supported by dynamics. Here we provide a comprehensive picture of this crossover. In our study, we show the detailed behaviour of the quasiparticle weights, that show an asymmetric cusp-like singularity in the effective mass as a function of field. We show that the effective mass increases monotonically as the metamagnetic transition is approached, and beyond the transition the effective mass decreases smoothly and monotonically for lower $U$, while for higher $U$ there is a sharp discontinuous decrease. The applied field gets renormalized to an effective field through the polarization of the medium (within DMFT) and via interaction effects.

We show that the lattice Kondo resonance at the Fermi level splits into two at large fields: the up and down components move away from the Fermi level and finally form a spin polarized band insulator. The shift of the band is not rigid due to the competition between the Kondo screening and the Zeeman effect. The hysteresis across the metamagnetic transition is used to find the ‘phase diagram’. Our calculations agree quantitatively with the NRG study of Bauer [27] and we regard this agreement as an important benchmark. The low field universal features of the spectral functions are carefully examined and adiabatic continuity to the non-interacting limit is demonstrated. We argue that the field induced metamagnetic transition is from a correlated paramagnetic metallic liquid to a band insulator, and in this sense is very different from the interaction-driven first order Mott transition, which is from a correlated metallic liquid to a correlated Mott insulator. We compare our theoretical result with the experimental one on liquid $^3$He and find good qualitative agreement.

The paper is organized as follows. We begin in section 2 with a brief description of the model. In section 3, we present our theoretical results and their analysis. We also compare our theory with the experimental results on liquid $^3$He. Finally, we conclude in section 4.

2. Model and formalism

The single band Hubbard model Hamiltonian describing correlated electrons in the presence of an external magnetic
field (the orbital contribution is neglected) is given by:

$$
\hat{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c}) + U \sum_i n_{i \uparrow} n_{i \downarrow} + \sum_{i \sigma} (\epsilon_i - h \sigma) n_{i \sigma}.
$$

(1)

The first term describes the kinetic energy of the non-interacting conduction (c) band due to nearest neighbour hopping $t$. The second term refers to the on-site repulsion $U$. The final term represents the orbital energy and the Zeeman splitting in an external magnetic field. For the particle–
hole symmetric (half-filled) case considered in this work, the orbital energy is given by $\epsilon_i = -U/2$. In the limit of large dimensions, $D \to \infty$, the hopping needs to be scaled as $t \propto t_0/\sqrt{D}$. We choose, for convenience, a hypercubic lattice, for which the non-interacting density of states is an unbounded Gaussian ($\rho_0(\epsilon) = \exp(-\epsilon^2/|t_0|^2)/(\sqrt{\pi}t_0)$). We set $t_0 = 1$ in the following calculation.

Within DMFT, which is exact in the limit of infinite dimensions, as is well known, the lattice model may be mapped to an effective single-impurity Anderson model with a self-consistent hybridization [7, 8]. The major simplification that occurs is that the self-energy and the vertex function become local and momentum-independent. In the presence of an external global magnetic field, the local, retarded Green’s function is given by

$$
G_\sigma(\omega, h) = H [\gamma_\sigma(\omega; h)]
$$

(2)

where $\gamma_\sigma(\omega; h) = \omega^+ + \epsilon_\sigma + \sigma h - \Sigma_\sigma(\omega, h)$, $H[z]$ is the Hilbert transform defined as

$$
H[z] = \int \frac{\rho_0(\epsilon)}{z - \epsilon} \, d\epsilon
$$

and $\Sigma_\sigma(\omega; h)$ is the spin-dependent local self-energy. The local Green’s function may be used to define a hybridization function $S(\omega; h)$ as

$$
S(\omega) = \gamma_\sigma(\omega; h) - \frac{1}{H[\gamma_\sigma(\omega; h)]}
$$

(3)

The hybridization function defines the host or the medium within which the impurity is embedded, and the non-interacting host Green’s function is then given by

$$
G_\sigma(\omega, h) = \frac{1}{\omega^+ - \epsilon_\sigma + \sigma h - S(\omega; h)}
$$

(5)

which is equivalent to using the Dyson equation

$$
G_\sigma^{-1}(\omega, h) = G_\sigma^{-1}(\omega, h) + \Sigma_\sigma(\omega, h).
$$

(6)

This host Green’s function is then used to construct a new impurity self-energy, which if substituted in equation (2) yields a new lattice Green’s function. Thus the solution within DMFT proceeds most easily in an iterative manner using equations (2)–(6) until self-consistency is achieved.

Although easily stated, constructing a new impurity self-energy for an arbitrary non-interacting host has remained a major bottleneck in the DMFT scheme. Various impurity solvers have been developed, the most important of which are quantum Monte Carlo, exact diagonalization, numerical renormalization group, diagrammatic perturbation theory based approaches etc. We employ the iterative perturbation theory (IPT) approach to solve the impurity problem within DMFT. The IPT is a very simple yet powerful diagrammatic perturbation theory based approach. It has been benchmarked extensively against more exact methods in the zero field half-filled Hubbard model problem. The agreement, though qualitative, is excellent. The main advantage of IPT is the ability it provides to capture real frequency dynamics, and hence transport on all frequencies, temperature scales and interaction strengths. For a more detailed comparison with other impurity solvers, we refer the reader to a previous article by one of the authors of the present work [16].

The zero temperature ($T = 0$) self-energy has the following form, consisting of the static Hartree contribution and the dynamical part:

$$
\Sigma_\sigma(\omega, h) = U \tilde{n}_\sigma + \Sigma_\sigma^{(2)}(\omega, h)
$$

(7)

where $\tilde{n}_\sigma = \int_{-\infty}^{\infty} d\omega \, D_\sigma(\omega)$ and $D_\sigma(\omega) = -\frac{1}{\pi} \text{Im} G_\sigma(\omega)$ is the spectral function of the host Green’s function. The local IPT self-energy $\Sigma_\sigma^{(2)}(\omega, h)$ which satisfies the Luttinger theorem automatically at half-filling is given by (this zero field algorithm has been discussed recently in detail [17])

$$
\Sigma_\sigma^{(2)}(\omega, h) = U^2 \int_{-\infty}^{\infty} d\omega' \, D_\sigma(-\omega; h) \times \left[ \chi^{\sigma\sigma}_{\uparrow}(\omega + \omega') f(\omega') + \chi^{\sigma\sigma}_{\downarrow}(\omega + \omega') f(-\omega') \right]
$$

(8)

where

$$
\chi^{\sigma\sigma}_{\uparrow}(\omega) = \int_{-\infty}^{\infty} d\omega' \, D_\sigma(\omega') D_\sigma(\omega + \omega') f(-\omega' - \omega')
$$

and $f(\omega) = \left[ e^{\beta \omega} + 1 \right]^{-1}$ is the Fermi function.

The magnetization can be calculated from

$$
m = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle
$$

(10)

where $\langle n_\sigma \rangle = \int_{-\infty}^{\infty} d\omega \, (\frac{1}{2} - \frac{1}{\pi}) \text{Im} G_\sigma(\omega)$.

3. Results and discussions

In this section we will discuss the results of our calculations so far on the effect of magnetic field on the Hubbard model at half-filling. Before discussing the finite field results, we will briefly review the well-known zero field results for the Hubbard model. At zero field, the system goes from a metal and shows Fermi liquid behaviour. There is a coexisting region between $U_0$ and $U_\text{C}$. The values of $U_0$ and $U_\text{C}$ for the hypercubic lattice are 3.67$t_u$ and 4.78$t_u$ [4, 5]. We are
Figure 1. Magnetization as a function of field for various $U/t_\epsilon$ values. The magnetization smoothly approaches the saturation value of 1 for $U < 1.4t_\epsilon$, while for $U > 1.4t_\epsilon$ a metamagnetic first order transition is seen. The magnetization jumps at a finite value of the field, which falls sharply with increasing transition is seen. The inset shows the same data as the main panel on a logarithmic field axis, so that the sharp decrease in the value is seen clearly.

Figure 2. Hysteresis is seen across the metamagnetic transition. We illustrate this for $U = 1.5t_\epsilon$ here. The dotted line is the actual obtained line when the parameter $h_m$ is continuously increased. The region where the susceptibility, $\chi = \partial m / \partial h$, becomes negative is excluded to obtain the hysteresis.

interested in the region below $U_c$. At zero field, the spectra show a universal scaling form in terms of $\omega_L$ (where $\omega_L = Zt_\epsilon$ and $Z$ is the quasiparticle weight).

We will begin with a discussion of the symmetry properties of the Green’s function and the associated self-energies. The following symmetry holds in the half-filled case:

$$ G(\omega; h) = -[G(-\omega; h)]^* $$

$$ \Sigma(\omega; h) = -[\Sigma(-\omega; h)]^*. $$

To see this, imagine carrying out the self-consistent DMFT iterations beginning with a symmetric hybridization function, as appropriate for the zero field case. Naturally, the resulting host Green’s function (equation (5)) will satisfy the above symmetries. The self-energies calculated through the IPT ansatz (equations (8) and (9)) would then also satisfy the same symmetries, as then would the full interacting Green’s function (equation (3)). One consequence of such a symmetry is that the quasiparticle weights $Z_\sigma$ would be spin-independent.

Rewriting equation (7) as $\Sigma_\sigma(\epsilon; h) = -\Sigma_\sigma(\bar{\epsilon}; \bar{h}) + \Sigma_\sigma^{(2)}(\epsilon; h)$, where $\bar{n} = \bar{n}_\uparrow - \bar{n}_\downarrow$ is a fictitious local moment (of the host/medium), and using $\epsilon_c = -U/2$ and $\bar{n} = 1$, we transform equation (2) as

$$ G_\sigma(\omega; h) = \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon) d\epsilon}{\omega^2 - \epsilon + \sigma(h + \frac{\epsilon}{2}\bar{n}) - \Sigma_\sigma^{(2)}(\omega; h)}. $$

We would like to mention a technical point here. We found that the IPT equations are ill-behaved for a fixed field. In other words, if we wish to find the value of the magnetization self-consistently through the iterative procedure, keeping the field fixed, we run into problems of convergence. An easy way to avoid this instability is to work with a fixed value of the composite number $h_m \equiv h + U\bar{m}/2$. The equations converge easily and a unique solution is found. The host Green’s functions can be then used to find $\bar{m}$, and the field value is obtained as $h = h_m - U\bar{m}/2$. A similar strategy was employed by Laloux et al [25] in their ED + DMFT approach, where they had to use a fixed magnetization to achieve convergence. The final value of the actual magnetization is found through equation (10).

Our results for magnetization are summarized in figure 1. The magnetization ($m$) is shown as a function of field ($h$) for increasing values of the interaction strength $U/t_\epsilon$. The magnetization smoothly approaches the saturation value of 1 for $U < 1.4t_\epsilon$, while for $U > 1.4t_\epsilon$ a metamagnetic first order transition is seen. The magnetization jumps at a finite value of the field $h_c$, which falls sharply with increasing $U/t_\epsilon$ (figure 3), and beyond $U/t_\epsilon = 2.2$ becomes unresolvably small.

Figure 3. The coexistence region (shaded) as obtained within IPT for the hypercubic lattice. At large $U \gtrsim 2.2 t_\epsilon$, the system is susceptible to being polarized for an infinitesimal field.
within the present approach. The jump size increases from 0 at $U_{bc} = 1.4t_s$ to a large value ($\sim 0.67t_s$) at $U = 2.1t_s$. The value of $U_{bc} = 1.4t_s$ does agree quantitatively with that obtained by Bauer [27] through NRG + DMFT. In the latter, a semi-circular density of states was chosen to represent the bare conduction band, $\rho_{bdm}^0 = 2\sqrt{D^2 - \epsilon^2/\pi} D^2$ with $D = 2t_s$. The value of $U_{bc}/t_s$ was found to be 2.64 in the NRG study [27], which corresponds to a $U_{bc}/D \simeq 1.32$, and thus the agreement with the IPT value (1.4) for the critical $U$ value provides our results an important benchmark. (1.4) This metamagnetic transition has been observed and studied previously within the GA and DMFT approaches. The low field state is a paramagnetic state, while the high field state beyond the transition is a polarized quasi-ferromagnetic state. As with the zero field case, the metamagnetic transition, being first order, would be accompanied by a hysteresis as the field is swept through a closed cycle across the transition. This is shown in figure 2 for $U = 1.5t_s$. Thus, there exists, for a range of $U$ values, a region in the $h_t - U$ plane that defines the ‘coexistence’ region, i.e. the region, where the paramagnetic metallic and the quasi-ferromagnetic insulating solutions coexist. This region may be identified through the bounds of the hysteresis curve for each $U$. In figure 3, the shaded region represents the coexistence region, and the solid lines are the equivalents of $U_{c1}$ and $U_{c2}$ for the finite field case. Indeed, Bauer [27] reports that the metallic solutions were impossible to obtain for $U/t_s \gtrsim 4.5$, which corresponds to $U/D \simeq 2.2$, which is the right boundary of the coexistence region in figure 3, and thus the coexistence region obtained within IPT for the hypercubic lattice agrees excellently with that of the NRG study. Since the quasi-ferromagnetic high field insulator is not, however, a Mott insulator, the term ‘equivalent’ above is not strictly precise. In fact, this two-phase region at finite field is not an ‘extension’ of the $U_{c1} - U_{c2}$ region in the $h = 0$ plane onto the finite $h$ plane. They do not merge onto each other and represent very different spinodal regions across different states.

We shift our focus to the quasiparticle weights or inverse effective mass. In figure 4, we show $Z$ as a function of field for various $U$ values, ranging from low $U$ at which metamagnetism is weak or absent, to a relatively high $U$, i.e. the strongly metamagnetic region, where the system is susceptible to being polarized even for an infinitesimal field.

At low $U = 1.0$, the magnetization increases smoothly with increasing field, and the effective mass decreases monotonically, approaching the bare mass at high fields. The behaviour of $m$ and $Z$ changes qualitatively for $U = 1.3t_s$: the effective mass displays a cusp, while the magnetization changes slope significantly. The cusp sharpens for $U = 1.5t_s$, while $Z$ suffers a discontinuous increase at the metamagnetic transition. At an even higher value, $U = 2.0$, both the magnetization and the effective mass display discontinuous changes at the transition. Thus the field dependence of magnetization and effective mass is very sensitive to the specific $U/t_s$ values under consideration.

The main advantage with the IPT approach used here is that we can study the real frequency dynamics in detail. We now proceed to elucidate the field dependence of the dynamics before and across the metamagnetic transition. We begin by exploring the universal scaling properties by carrying out a low frequency Fermi liquid analysis. In the metallic phase of interest, the real part of self-energy may be expanded about the Fermi level to first order in $\omega$:

$$\text{Re} \Sigma^{(2)}(\omega, h) = \text{Re} \Sigma^{(2)}(0, h) + \left(1 - \frac{1}{Z(\omega)}\right)\omega$$

(14)

where $Z(\omega) = |1 - \partial \Sigma^R(\omega; h)/\partial \omega|^{-1}$. For the half-filled case considered in this paper, $Z_\uparrow = Z_\downarrow$ (as argued before), hence we drop the spin subscript. The imaginary part of the self-energy remains Fermi liquid like ($\sim O(\omega^2)$) because of the structure of the IPT equations (equations (8) and (9)). A finite imaginary part can be acquired by the self-energy only at finite temperatures in this approach. Substituting the above equation (13), the spectral function $D_\sigma = -\text{Im} \Sigma(\omega/\pi)$, is obtained as

$$D_\sigma(\omega, h) \rightarrow \rho_0(\omega + \sigma h^{\text{eff}})$$

(15)

where $\sigma = \omega/\omega_{\text{L}}$ (with $\omega_{\text{L}} = Z(h_t)s$) and the spin-independent (because of the symmetries, equation (12)) effective field is given by

$$h^{\text{eff}} = h + \frac{U}{2} \tilde{m} - \sigma \text{Re} \Sigma^{(2)}(0, h).$$

(16)

The above equation (15) is the renormalized non-interacting limit of the full spectral function. Given the above form of the spectral function, it is easy to see that adiabatic continuity to the non-interacting limit is achieved provided the real part of the self-energy can be expanded as in equation (14). Using equation (15), we can infer that the spin-summed spectra would also be a universal function of $\tilde{\omega}$ for a fixed $h^{\text{eff}}$. Whether...
the full field-dependent spectra satisfy adiabatic continuity and scaling may be tested through equation (15).

The dependence of effective field \( h_{\text{eff}} \) on the applied field is shown in figure 5 for various \( U \) values. The metamagnetic transition is reflected in the effective field as well. A careful examination of the contribution to the effective field indicates that the discontinuity is present not only in the real part of \( \Sigma^{(2)}(0; h) \) but also in the host magnetization \( \bar{m} \).

The spectra for various \( U/t^* \) plotted as a function of \( \omega/\omega_L \). All the \( U > 0 \) spectra are seen to be identical to that of the non-interacting case, near the Fermi level, as shown in figure 6. Also shown in the same graph is the non-interacting density of states (DOS) for a field of \( h = 0.3t^* \) and \( Z = 1 \). The universal form is seen to be identical to the non-interacting spectral function for the same parameters (see text for discussion).

We now move on to the field dependence of the spectral functions for a given interaction strength. In the absence of clear metamagnetism (\( U = 1.0 \)), the evolution of the spectral function with field is very similar to a non-interacting case, as expected. The density of states at the Fermi level continues to decrease with increasing field, until the up and down spin bands move so far from the Fermi level that a band insulator is obtained. This is shown in the upper panel of figure 7. The lower panel of the same figure represents \( U = 1.3 \), which is close to the onset of metamagnetism. Again, the behaviour is similar, albeit the decrease of the density of states at the Fermi level with increasing field is more pronounced. We add here that the IPT results for the field dependence of the spectral functions are not in agreement with the NRG + DMFT results of Bauer et al [27]. In the latter, the spectral function seems to be pinned at the Fermi level until the metamagnetic transition, whence there is a sudden drop in the density of states. We do not understand this difference from NRG completely, but speculate that this disagreement could be due to the non-conserving nature of IPT.

The evolution of the spectral function for \( U = 1.5 \) and 2.0 (figure 8) with field is quite dramatic, reflecting the metamagnetic transition. The spin bands shift rapidly with field, and for the critical field at which the transition happens, the shift from a metallic to a quasi-ferromagnetic insulator takes place. Though the insulating state is reminiscent of a Mott insulator, it is actually far from being one. The two ‘Hubbard bands’ are just the two spin bands shifted away from the Fermi level, and broadened to an extent that they just resemble a non-interacting Gaussian DOS. In fact, the large field spectral function may be deduced from the large field asymptote of equation (13). At large field \( h \sim t^* \), the effective field becomes comparable to or larger than the largest scale in the problem, i.e. \( U \) in strong coupling. This is because, for \( h \simeq t^* \), the magnetization saturates, \( \bar{m} \to 1 \), hence the effective field becomes at least \( h + U/2 \). The real part of the second order self-energy contributes \( 1/U \) at frequencies
Figure 8. The upper (lower) panel represents the spectral function for $U = 1.5$ ($U = 2.0$) and various field values plotted against the bare frequency, $\omega / t_s$.

Figure 9. The splitting between the up and down spin bands is plotted against field for various $U$ values.

Figure 10. Comparison of the experimental magnetization in liquid $^3$He (filled circle) with theory (solid line).

$\omega \simeq U$, because $\Sigma^{(2)}(\omega) \sim 1/\omega$ at large frequencies. Thus from equation (13) the large field spectra must be simply given by $[\rho_0(\omega + h_{\text{eff}}) + \rho_0(\omega - h_{\text{eff}})]/2$. This is just a sum of two Gaussians each centred around $\pm h_{\text{eff}}$, respectively. Indeed, from figure 5, we see that for $U = 2.0$, the value of the effective field is $\sim 2.5$ for a field of $h = 0.5$; and the lower panel of figure 8 shows that the two ‘Hubbard bands’ are centred around $\pm 2.5$. This indicates that at high field all correlation effects are lost, and the ‘Hubbard bands’ are nothing but the bare density of states shifted away from the Fermi level, and thus the insulator at high fields is just a band insulator.

The split between the up and down spin bands may be quantified, and is shown in figure 9 for various $U$ values. The field induced shift of the spin bands is seen to be highly nonlinear and indeed even discontinuous for $U = 1.5$ and 2.0, naturally at the metamagnetic transition. In the non-interacting case this split is a rigid Zeeman shift. But in the interacting case the shift is not rigid at all. In the periodic Anderson model (appropriate for heavy fermion systems), the effect of magnetic field in the Kondo lattice regime is similar (without metamagnetism), and it has been argued that the non-rigid shift is due to the competition between Kondo screening of the local moments (whose effect is to quench the local moments) and the Zeeman coupling (whose effect is to polarize the local moments). In the present case, since the lattice Hubbard model is mapped onto the single-impurity Anderson model within DMFT, similar arguments must apply. And it is possibly this competition here which is ultimately responsible for the first order metamagnetic transition. We see that the field induced transition is very different from the temperature induced transition, or the pure interaction induced Mott transition at zero field. In the latter especially, as one approaches $U_{c2}$ from the metallic side, the Fermi liquid scale $Z_{t_s}$ vanishes continuously, and upon crossing into the Mott insulator side, a large and finite gap appears discontinuously in the density of states. At $U_{c1}$ the reverse happens, i.e. the gap in the Mott insulator vanishes continuously on decreasing $U$, and on crossing $U_{c1}$ a Fermi liquid with a finite quasiparticle weight $Z$ is found. At finite field, however, neither the Fermi liquid scale nor the gap vanishes at the metamagnetic transition.

Finally we would like to compare our theory with experiments. The experimentally measured magnetization [24] as a function of effective field at temperatures $T \sim 70–90$ mK is shown in figure 10 as filled circles. The authors of the experimental paper concluded that the first order metamagnetic transition scenario proposed by Vollhardt [21] cannot be applicable to the case of liquid $^3$He, since metamagnetism is absent in the experimental data, although a slight metamagnetic kink can be distinguished at a field of about 180 T. We argue that the applicability of the half-filled Hubbard model cannot be ruled out yet, since as our figure 1 shows the magnetization can be a smooth function of the field for low to intermediate interaction strengths. According to Vollhardt [21], $U$ is typically about 15 K for $^3$He, while the parameter $U/E_F \sim 0.8$, where $E_F$ is the Fermi energy. So this does seem to be an intermediate coupling scenario. Indeed, if we superimpose the calculated magnetization for $U = 1.0 t_s$ onto the experimental data (after a multiplicative scaling of the field axis), we see surprisingly good agreement. The GA yields a discontinuous metamagnetic transition for rather weak interactions, while we find that metamagnetism does
not develop until a reasonably strong interaction strength of $U \gtrsim 1.3 t_*$ within the IPT + DMFT approach employed here.

4. Conclusions

In this paper, we have studied the effect of magnetic field on correlated electron liquids within the framework of the half-filled Hubbard model using a dynamical mean field theory. We compute the single particle dynamics, magnetization and other zero temperature properties. For intermediate $U$ values, we find a first order itinerant metamagnetic transition, in agreement with earlier theoretical studies. An important benchmark for our study was the agreement with the NRG + DMFT calculations [27] regarding the onset of metamagnetism and the coexistence region in the $h$–$U$ plane.

We conjecture that the first order metamagnetic transition is a result of the competition between Kondo screening and Zeeman coupling. The metamagnetic transition is found to be very different in nature from the zero field interaction driven Mott transition. Beyond $U = 2.2 t_*$, we find that even an (numerically) infinitesimal field is sufficient to push the system from a zero field paramagnetic state to a polarized quasi-ferromagnetic state with a substantial magnetization. Finite temperature transport and dynamics studies would be instrumental in furthering an understanding of this transition.

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