Magnetic Field Effects on Quasiparticles in Strongly Correlated Local Systems

A.C. Hewson, J. Bauer and W. Koller
Department of Mathematics, Imperial College, London SW7 2AZ. UK
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We show that quasiparticles in a magnetic field of arbitrary strength $H$ can be described by field dependent parameters. We illustrate this approach in the case of an Anderson impurity model and use the numerical renormalization group (NRG) to calculate the renormalized parameters for the levels with spin $\sigma$, $\tilde{\varepsilon}_{d,\sigma}(H)$, resonance width $\tilde{\Delta}(H)$ and the effective local quasiparticle interaction $\tilde{U}(H)$. In the Kondo or strong correlation limit of the model the progressive de-renormalization of the quasiparticles can be followed as the magnetic field is increased. The low temperature behaviour, including the conductivity, in arbitrary magnetic field can be calculated in terms of the field dependent parameters using the renormalized perturbation expansion. Using the NRG the field dependence of the spectral density on higher scales is also calculated.

I. INTRODUCTION

Electrons in strongly correlated systems are particularly sensitive to the application of magnetic fields. One reason is that strong correlations are usually a consequence of the interaction of electrons with enhanced spin fluctuations, and these fluctuations couple strongly to a magnetic field. Another reason is that there is a low temperature scale $T^*$ ($T^* \ll T_F$) induced which plays the role of an effective Fermi temperature $T_F$. The effects of a magnetic field $H$ in general depend on the ratio of the two energy scales $\mu_B H$ and $k_B T_F$. In a weakly correlated metal $\mu_B H/k_B T_F \ll 1$, but in a strongly correlated system the relevant ratio is $\mu_B H/k_B T^*$, which can be of order unity. This sensitivity means that a magnetic field is an important tool in the experimental investigation of strongly correlated metallic systems, such as magnetic impurities, quantum dots, heavy fermions and transition metal oxides.

In this paper we concentrate mainly on the effects of a magnetic field on the quasiparticles in the Fermi liquid regime for various models of strongly correlated metals. In particular we develop an approach, based on a combination of the numerical renormalization group (NRG) and renormalized perturbation theory (RPT). This approach gives a comprehensive picture of the behaviour of quasiparticles in magnetic fields of arbitrary strength, such that we can follow the renormalization or de-renormalization of the quasiparticles as the magnetic field strength is changed. In this paper we concentrate on developing the approach for the single impurity Anderson model (SIAM), as a model of magnetic impurities and quantum dots. This prepares the way for generalizing the approach to lattice models for transition metal oxides and heavy fermion materials, using dynamical mean field theory (DMFT), which will be the subject of a subsequent paper.

II. QUASIPARTICLES AT $T = 0$ WITH ZERO MAGNETIC FIELD

The generic model for strongly correlated local systems, such as magnetic impurities in a host metal or a quantum dot coupled to an electron reservoir, is the Anderson model. The Hamiltonian for this model is

$$
H_{AM} = \sum_{\sigma} \varepsilon_{d,\sigma} d_{\sigma}^\dagger d_{\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{k,\sigma} (V_{kd,\sigma} c_{k,\sigma} + V_{kd,\sigma}^* c_{k,\sigma}^\dagger d_{\sigma}) + \sum_{k,\sigma} \varepsilon_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma},
$$

where $\varepsilon_{d,\sigma} = \varepsilon_d - \sigma g \mu_B H/2$ is the energy of the localized level at an impurity site or quantum dot in a magnetic field $H$, $U$ the interaction at this local site, and $V_k$ the hybridization matrix element to a band of conduction electrons with energy $\varepsilon_k$. When $U = 0$ the local level broadens into a resonance, corresponding to a localized quasi-bound state, whose width depends on the quantity $\Delta(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \varepsilon_k)$. It is usual to consider the case of a wide conduction band with a flat density of states where $\Delta(\omega)$ becomes independent of $\omega$ and can be taken as a constant $\Delta$.

The low energy behaviour of this model can be expressed in terms of the renormalized quasiparticles of a local Fermi liquid, which is described by a renormalized version of the same model:

$$
\tilde{H}_{AM} = \sum_{\sigma} \tilde{\varepsilon}_{d,\sigma} d_{\sigma}^\dagger d_{\sigma} + \tilde{U} : n_{d,\uparrow} n_{d,\downarrow} :
+ \sum_{k,\sigma} (\tilde{V}_{kd,\sigma} c_{k,\sigma} + \tilde{V}_{kd,\sigma}^* c_{k,\sigma}^\dagger d_{\sigma}) + \sum_{k,\sigma} \tilde{\varepsilon}_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma},
$$

where the colon brackets indicate that the expression within them must be normal-ordered. This Hamiltonian corresponds to the low energy fixed point of the Wilson numerical renormalization group transformation of the discretized Anderson and Kondo models, with the leading irrelevant terms. The advantage of describing the fixed point in this way, as a renormalized Anderson model rather than as a strong coupling fixed point of the Kondo model, even in the strong correlation or Kondo...
The limit, is that it clearly brings out the 1-1 correspondence of the low-lying single particle excitations with those of the non-interacting model. Furthermore, it is applicable in all parameter regimes, from weak to strong coupling and for all occupation values for the local site. The parameters $\tilde{\varepsilon}_d$, $\Delta$, and $\bar{U}$ define the quasiparticles of this renormalized model, and a simple direct procedure for calculating these parameters using the NRG has been given earlier. In terms of these parameters the Friedel sum rule \cite{10,11}, which gives the total occupation of the d-orbital at the impurity site $n_d$ for $T = 0$ in the wide band limit, is

$$n_d = 1 - \frac{2}{\pi} \tan^{-1} \left( \frac{\tilde{\varepsilon}_d}{\Delta} \right).$$

(3)

In the wide band limit the renormalized parameters, $\tilde{\varepsilon}_d$, $\Delta$, and $\bar{U}$, can be expressed as functions of two independent 'bare' parameters, which can be taken to be $U/\pi\Delta$ and $\varepsilon_d/\pi\Delta$. Some typical plots of the renormalized parameters as a functions of these variables were presented in the earlier work. An alternative way of presenting the results is in terms of just one of these variables, $U/\pi\Delta$, and the occupation of the impurity levels $n_d$, which gives a global picture over the various regimes of the model.

In figures 1(a), 1(b) and 1(c) we present results for the ratios, $\Delta/\Delta$, $\tilde{\varepsilon}_d/\varepsilon_d$ and $\bar{U}/U$, where $\varepsilon_d = \varepsilon_d + U/2$, which give a measure of the degree of renormalization of these parameters for the 'bare' values of $U/\pi\Delta = 0.5, 1, 1.5, 2, 2.5, 3$. In the empty ($n_d \rightarrow 0$) and full ($n_d \rightarrow 2$) regimes all the parameters approach their unrenormalized values so these ratios tend to unity. The renormalizations are the most pronounced in the region $n_d \approx 1$. In the almost localized (Kondo) regime, $n_d \approx 1$, $U/\pi\Delta > 2$, there is only one energy scale, the Kondo temperature $T_K$, such that $\varepsilon_d \approx 0$ and $\bar{U} = \pi\Delta = 4T_K$.

The impurity density of states for the non-interacting quasiparticles $\tilde{\rho}_d(\omega)$ at $T = 0$ is given by

$$\tilde{\rho}_d(\omega) = \frac{\Delta/\pi}{(\omega - \varepsilon_d)^2 + \Delta^2},$$

(4)

and in the localized regime corresponds to a Kondo resonance of half-width $\Delta = 4T_K/\pi$ at the Fermi level, where the Kondo temperature is defined in terms of the impurity spin susceptibility $\chi_s$ at $T = 0$ via $T_K = (g\mu_B)^2/4\chi_s$.

As in the general Fermi liquid theory, the linear coefficient of the specific heat for the impurity can be expressed simply in terms of the quasiparticle density of states at the Fermi level, and is given by

$$\gamma_d = \frac{2\pi^2}{3} \tilde{\rho}_d(0).$$

(5)

Exact expressions for impurity spin and charge susceptibilities, $\chi_s$ and $\chi_c$, in terms of the renormalized parameters for $T = 0$ are

$$\chi_s = \frac{1}{2} \tilde{\rho}_d(0)(1 + \bar{U}\tilde{\rho}_d(0)), \quad \chi_c = \frac{1}{2} \tilde{\rho}_d(0)(1 - \bar{U}\tilde{\rho}_d(0)).$$

(6)

These results can be derived using the renormalized perturbation approach working simply only up to first order in $\bar{U}$ (see also the Appendix here).

It is interesting to note that these Fermi liquid results
apply even in the limit \( \varepsilon_d \to -\infty, U \to \infty \), when the charge fluctuations are completely suppressed and the Kondo scale \( T_K \to 0 \). In this limit \( \bar{U}_d(0) \to 1 \) and \( \bar{\rho}_d(\omega) \to \delta(\omega) \) corresponding to the low energy excitations of an isolated spin. If the finite temperature Fermi distribution function is included in the calculations leading to \( \chi_c \) and \( \chi_s \) in equation (6), then in this limit \( \chi_c \to 0 \), and \( \chi_s \to (g\mu_B)^2/4k_B T \), the Curie law for a localized magnetic moment.

So far we have assumed a repulsive interaction \( U > 0 \), but the formulae are equally applicable to the case of an attractive interaction \( U < 0 \). In this case, however, except at the particle-hole symmetric point, the renormalized parameters behave quite differently as a function of \( |U|/\pi \Delta \) and \( n_d \). In figures 2(a), 2(b) and 2(c), we present results for the ratios, \( \Delta/\Delta, \bar{\varepsilon}_d/\varepsilon_d \), and \( \bar{U}/U \), for values of \( U/\pi \Delta = -(0.5, 1, 1.5, 2, 2.5, 3) \).

In comparing the results in figure 2(a)(b) and (c) with the corresponding results in figure 1 (a)(b) and (c), it can be seen that, irrespective of the sign of \( U \) all the parameters converge to their bare values in limits \( n_d \to 0 \) and \( n_d \to 2 \) and the values of \( \Delta/\Delta \) and \( \bar{U}/U \) are the same at the symmetric point \( n_d = 1 \), they are remarkably different elsewhere. In the range \( 0.5 < n_d < 1.5 \), \( \Delta/\Delta \) and \( \bar{U}/U \) for \( U < 0 \) are remarkably flatter than the corresponding results for \( U > 0 \), especially for large values of \( |U| \). The ratios \( \bar{\varepsilon}_d/\varepsilon_d \) and \( \bar{U}/U \) for \( U < 0 \) do not increase monotonically with increase of \( |n_d - 1| \), as they do in the corresponding \( U > 0 \) results. The ratio \( \bar{U}/U \) develops a sharp peak with values such that \( \bar{U} > U \) and is completely different from the positive \( U \) counterpart. The ratio \( \bar{\varepsilon}_d/\varepsilon_d \) is also completely different and is greater than, or equal to, unity over the whole range, developing a similar peak to that for \( \bar{U}/U \). At the particle-hole symmetric point, \( n_d = 1, \bar{\varepsilon}_d = 0, \) and \( \bar{\varepsilon}_d = 0 \), so the ratio \( \bar{\varepsilon}_d/\varepsilon_d \) is not defined. In the positive \( U \) case, the ratio tends to 0 for large \( |U| \) and to 2 in the negative \( U \) case.

The main applications of the Anderson model to magnetic impurities and quantum dots are for the positive \( U \) case, though the negative \( U \) model has some limited application as an effective model for some locally coupled electron-phonon systems, where a local attraction is induced through the exchange of a virtual phonon. However, in the next section we shall exploit the negative \( U \) model here by using spin-isospin symmetry to transform it into a model with positive \( U \) with particle-hole symmetry in the presence of a magnetic field. The restriction to the \( n_d = 1 \) particle-hole symmetric case will not be a serious limitation because in the strong correlation/local moment limit the renormalized level rapidly approaches the Fermi level for large \( U \), \( \bar{\varepsilon}_d \to 0 \), and hence via the Friedel sum rule \( n_d \to 1 \). In this particle-hole symmetric case there is only one energy scale for a given \( U/\pi \Delta \), which we denote by \( T^* \) and define by \( T^* = \pi \Delta/4 \); it is such that \( T^* \to T_K \) in the Kondo regime \( U/\pi \Delta > 2 \).

FIG. 2: Plots of the renormalized parameters for the Anderson model, (a) \( \Delta/\Delta \), (b) \( \bar{\varepsilon}_d/\varepsilon_d \), and (c) \( \bar{U}/U \), as a function of the occupation of the impurity site \( n_d \), for values of \( U/\pi \Delta = -(0.5, 1.0, 1.5, 2.0, 2.5, 3.0) \).

III. QUASIPARTICLES AT \( T = 0 \) WITH ARBITRARY MAGNETIC FIELD \( H \)

The spin-isospin transformation which formally eliminates the magnetic field term in the symmetric model is defined by

\[
c_{d\uparrow} \to c_{d\uparrow}^\dagger, \quad c_{d\downarrow}^\dagger \to c_{d\downarrow}
\] (7)
with the requirement \( \epsilon_{-k} = -\epsilon_k \) with \( V_{-k}^* = -V_k \).

With this transformation for the symmetric model with \( U > 0 \) and \( \tilde{\epsilon}_d = 0 \) in the presence of a magnetic field \( H \) at the impurity site gets mapped into the model with an interaction \(-U\), and no magnetic field but with \( \tilde{\epsilon}_d = g\mu_B H/2 = h \). The spin/charge susceptibilities for the positive \( U \) symmetric model in a magnetic field are then given by the charge/spin susceptibilities of the model with a negative \( U \). The magnetic field dependent parameters \( \Delta(h), \tilde{\epsilon}_{d,\sigma}(h) \) and \( \tilde{U}(h) \), for the \( U > 0 \) model then correspond to \( \tilde{\Delta}(h), -\sigma\tilde{\epsilon}_{d}(h) \) and \( -\tilde{U}(h) \) for the corresponding negative \( U \) model with \( \tilde{\epsilon}_d = h \). The Friedel sum rule is still applicable to each spin component from which the induced impurity magnetization \( M(h) \) at \( T = 0 \) can be deduced,

\[
m(h) = \frac{M(h)}{g\mu_B} = \frac{1}{2}(n_{d,\uparrow} - n_{d,\downarrow}) = \frac{1}{\pi} \tan^{-1}\left(\frac{\tilde{\epsilon}_d(h)}{\Delta(h)}\right),
\]

from the two parameters \( \tilde{\epsilon}_d(h) \) and \( \tilde{\Delta}(h) \) that characterize the non-interacting quasiparticles. The quasiparticle density of states for the spin up and spin down electrons is given by

\[
\rho_{d,\sigma}(\omega, h) = \frac{\tilde{\Delta}(h)/\pi}{(\omega - \sigma\tilde{\epsilon}_d(h))^2 + \Delta^2(h)},
\]

and the field dependent spin and charge susceptibilities at \( T = 0 \) are given by

\[
\chi_s(h) = \frac{1}{2} \rho_{d}(0, h)(1 + \tilde{U}(h)\rho_{d}(0, h)),
\]

\[
\chi_c(h) = \frac{1}{2} \rho_{d}(0, h)(1 - \tilde{U}(h)\rho_{d}(0, h)).
\]

As \( \rho_{d,\sigma}(0, h) \) is independent of the spin state we can drop the spin index \( \sigma \).

As \( \tilde{\epsilon}_{d,\sigma}(h) \) is entirely magnetic field driven it is convenient to write it as \( \tilde{\epsilon}_{d,\sigma}(h) = h\tilde{q}(h) \), then \( 2h\tilde{q}(h) \) is the Zeeman splitting of the impurity levels for the non-interacting quasiparticles.

Using these results we can reinterpret the renormalized parameters in figures 2(a), (b) and (c) for the \( U < 0 \) model as \( \tilde{\Delta}(h)/\Delta, \tilde{q}(h) \) and \( \tilde{U}(h)/U \) for the \( U > 0 \) model as functions of the variable \( 2m(h) + 1 \), which replaces the \( n_d \). The fact that \( \tilde{\epsilon}_{d}/\tilde{\epsilon}_{d} \) in figure 2(b) approaches the value 2 as \( n_d \to 1 \) in the strong correlation limit can now be interpreted as \( \tilde{q}(h) \to 2 \) for \( h \to 0 \), which is equivalent to the Wilson ratio \( R = 4\pi\chi_s/3(g\mu_B)^2\gamma_{\text{imp}} = 2 \) for the strongly renormalized quasiparticles in zero field, which is enhanced compared with the free electron value \( R = 1 \). In figure 2(c) the sharp rise in \( U/U \) on reducing \( n_d \) from the value \( n_d = 2 \), can be interpreted as the enhancement of the effective interaction \( \tilde{U}(h) \), as the magnetization is reduced from the saturated value, \( m_{\text{sat}} = 1/2 \). As the applied magnetic field is reduced from the regime \( h > U \), spin fluctuations increase and enhance the effective interaction \( \tilde{U} \), as in the random phase approximation (RPA), above the bare value \( U \) (we will see this more explicitly later). As the magnetic field is further reduced the many-body correlations are increasingly effective in screening the impurity so that \( \tilde{U}(h) \) decreases from an enhanced value greater than \( U \) to a value \( 4T_K \) as \( h \to 0 \) when \( U > 2\pi\Delta \).

In figure 3 we give a more conventional plot of the renormalized parameters as a function of the natural logarithm of the magnetic field, \( \ln(h/T^*) \), for the strong coupling case \( U/\pi\Delta = 3 \), where \( T^* = \pi\Delta(0)/4 = 2.00 \times 10^{-2} = T_K \), in agreement to within 0.5% with formula\(^{13} \) for \( T_K \) for this model, \( T_K = \sqrt{(U/2)e^{-\pi U/8\Delta + \pi\Delta/2U}} \). We can follow the progressive de-renormalization of the quasiparticles as the strong correlation effects are suppressed as the magnetic field is increased. Initially the quasiparticle interaction \( \tilde{U}(h) \) increases and can reach values such that \( \tilde{U}(h) \) is greater than the bare interaction \( U \). This does not imply, however, that the interaction effects are becoming stronger. The effects of the interaction on the low energy scale depend upon the combination, \( \tilde{U}(h)\rho_{d}(0, h) \), and \( \rho_{d}(0, h) \) falls off rapidly with \( h \) as \( \tilde{\epsilon}_d(h) \) moves away from the Fermi level. The Wilson ratio \( R(h) = 1 + \tilde{U}(h)\rho_{d}(0, h) \) is a measure of this combination of factors and for the Kondo model it is known from Bethe ansatz calculations\(^{14} \) that \( R(h) = 2 \) is independent of \( h \). This can be seen to be the case in the results for \( R(h) \) shown in figure 3 when the parameters
correspond to the localized or Kondo regime. The localized model, however, is only valid when the charge fluctuations are completely suppressed. For very large field values \( h > U \) local charge fluctuations can be induced by the magnetic field and, as this regime is approached, \( R(h) \) makes a crossover to the value \( R = 1 \) for non-interacting electrons. The combination \( \tilde{U}(h) \tilde{\rho}_d(0, h) \) can be seen to decrease monotonically with increase of \( h \).

Equation (14) for the susceptibility \( \chi_s(h) \) has a term in \( \tilde{U}(h) \). However, the susceptibility can also be derived by differentiating the expression (12) for the magnetization which depends explicitly only on the variables \( \tilde{\varepsilon}_d(h) \) and \( \tilde{\Delta}(h) \). Hence the value of \( \tilde{U}(h) \) is not independent of the other two parameters and we can derive a relation between them,

\[
1 + \tilde{U}(h) \tilde{\rho}_d(0, h) = \frac{\partial \tilde{\varepsilon}_d(h)}{\partial h} - \frac{\tilde{\varepsilon}_d(h)}{\tilde{\Delta}(h)} \frac{\partial \tilde{\Delta}(h)}{\partial h}.
\]

The proof that equation (14) for the susceptibility is exact depends on a Ward identity, so the relation (15) we have derived must be an alternative statement of this identity. In terms of \( \tilde{\eta}(h) = \tilde{\varepsilon}_d(h)/h \) it becomes

\[
1 + \tilde{U}(h) \tilde{\rho}_d(0, h) = \frac{\partial \tilde{\eta}(h)}{\partial h} + h \frac{\partial \tilde{\eta}(h)}{\partial h} - \frac{h \tilde{\eta}(h)}{\tilde{\Delta}(h)} \frac{\partial \tilde{\Delta}(h)}{\partial h}.
\]

For \( h = 0 \) it implies that \( \tilde{\eta}(0) = R(0) \), which can be seen in the results in figure 3.

Mean field theory can also be interpreted in terms of renormalized parameters with \( \tilde{\varepsilon}_d(h) = h + U m_{\text{MF}}(h), \tilde{\Delta}(h) = \Delta, \) where \( m_{\text{MF}}(h) \) is the mean field magnetization. These parameters are substituted into equation (9), and \( m_{\text{MF}}(h) \) is determined self-consistently. From equation (16) we can deduce the corresponding value of \( \tilde{U}(h) \) which gives

\[
\tilde{U}(h) = \frac{U}{1 - U \tilde{\rho}_{\text{MF}}(0, h)},
\]

where \( \tilde{\rho}_{\text{MF}}(h, \omega) \) is the quasiparticle density of states with the mean field parameters. This result corresponds to the enhancement of the susceptibility that one finds from the random phase approximation. If the magnetic field is reduced from a large value \( h > U \) then \( \tilde{\rho}_{\text{MF}}(0, h) \) decreases and so \( \tilde{U}(h) \) increases. This is precisely what is seen in the large \( h \) regime in the results in figure 3, as well as those shown earlier in figure 2(b).

In figure 4 we plot the magnetization derived from these parameters for \( U/\pi \Delta = 3 \) as a function of \( \ln(h/T^*) \) using equation (16). We also give the magnetization deduced from the Bethe ansatz results for the Kondo model for comparison together with the value of \( R(h)/4 \). There is complete agreement with the results of the Kondo model, up to and just beyond the point at which local charge fluctuations are induced by the magnetic field, where \( R(h)/4 \) begins to decrease significantly from its strong correlation value 0.5. The ratio \( \tilde{\varepsilon}_d(h)/\tilde{\Delta}(h) \) must be a universal function of \( h/T_K \) for the Kondo regime. For \( h > T_K \) we have the asymptotic form \( 1/2 - m(h) \sim 1/4 \ln(h/T_K \Delta^*) \), so from equation (16), in this regime the ratio \( \tilde{\varepsilon}_d(h)/\tilde{\Delta}(h) \propto \ln(h/T_K) \). In figure 5 we plot the ratio \( \tilde{\varepsilon}_d(h)/\tilde{\Delta}(h) \) against \( \ln(h/T^*) \), for \( U/\pi \Delta = 5 \), which is well in the Kondo regime so \( T^* = T_K \). It can be seen this ratio is proportional to \( \ln(h/T_K) \) for a significant range of magnetic field values for \( h > T_K \), before the effects of the field induced charge fluctuations take over. Due to the charge fluctuations, the approach to saturation is much more rapid for the Anderson model than for the Kondo model, once \( h \) exceeds \( U \), as can be seen clearly in figure 4.

A similar plot of the magnetization \( m(h) \) against field on a logarithmic scale is shown in figure 6 for a weak correlation case \( U/\pi \Delta = 0.25 \). In this regime it is more appropriate to compare the results with mean field theory. The mean field results for the same parameters are also given in figure 6 (dashed line) and can be seen to be in good agreement. Also shown is the Wilson ratio \( R(h)/4 \), which is only weakly enhanced at \( h = 0 \), \( R(0) = 1.244 \), and makes a slow crossover to that for non-interacting electrons for \( h \sim \Delta \).

In figure 7 we give the magnetization \( m(h) \) against \( h/T^* \) for the more realistically realizable magnetic field regime \( 0 < h < 2.5T^* \) for a strong correlation case \( U/\pi \Delta = 3 \), using the renormalized parameters in equation (9). Points (×) corresponding to Bethe ansatz results for the Kondo model, are included for comparison and can be seen to be in complete agreement with those for the Anderson model in this regime. The results for \( m(h) \) for the weak coupling case \( U/\pi \Delta = 0.25 \)
are also shown in figure 7 together with the corresponding mean field theory results (dashed line). The $T^*$’s for the strong and weak correlation cases are very different, $T^*(3)/T^*(0.25) = 0.0827$, so the energy scales are very different but, relative to these scales, $m(h)$ increases initially more slowly with $h$ in the weak correlation case but approaches saturation more rapidly. The mean field results $U/\pi\Delta = 0.25$ also give a good approximation to $m(h)$ for $U/\pi\Delta = 0.25$ over this range.

Also shown in figure 7 are the values of $R(h)/4$ for the strong correlation case $U/\pi\Delta = 3$. It can be seen that there is a 5% reduction in $R(h)$ over this range to $h = 2.5T_K$, indicating some evidence of charge fluctuations beginning to contribute to the specific heat coefficient $\gamma_d(h)$ for intermediate field values, but having little effect on the magnetization. The localized model gives $R(h) = 2$ for all $h$, implies that $\tilde{U}(h) = 1/\tilde{\rho}_d(0, h)$. From this result, and equations (10) and (9), the ratio $\tilde{U}(h)/\pi\Delta(h)$ for the localized model can be expressed entirely in terms of the magnetization and is such that $\tilde{U}(h)/\pi\Delta(h) = 1/\cos^2(\pi m(h))$. For $h = 0$, this corresponds to the strong correlation results $\tilde{U}(0)/\pi\Delta(0) = 1$, as $m(0) = 0$, and for very large fields where $m(h) \to 1/2$ as $h \to \infty$, it gives $\tilde{U}(h)/\pi\Delta(h) \to \infty$, corresponding to the fact that charge fluctuations can only be completely suppressed if $U$ is infinite. In figure 8 we plot the ratio $\tilde{U}(h)/\pi\Delta(h)$ as a function of $h/(\pi T^*)$ for $U/\pi\Delta = 3, 5$, and compare the results with $1/\cos^2(\pi m(h))$, where $m(h)$ is calculated from the Bethe ansatz results for the Kondo model. It can be seen that the large peak in $\tilde{U}(h)/\pi\Delta(h)$ develops as $h$ increases, because it closely follows the result for the localized model $1/\cos^2(\pi m(h))$, and then falls back in very large fields to the unrenormalized ratio $U/\pi\Delta$. The results for $U/\pi\Delta = 5$ follow the form for the localized model $1/\cos^2(\pi m(h))$, implying $R(h) = 2$, for a greater range of $h$ than for the case $U/\pi\Delta = 3$, resulting in a more pronounced peak.

IV. LOW TEMPERATURE THERMODYNAMICS IN AN ARBITRARY MAGNETIC FIELD

We can generalize some of the results in the preceding section to calculate the leading temperature dependence in the presence of an arbitrary magnetic field. For in-
FIG. 8: The ratio $\tilde{U}(h)/\pi\Delta(h)$ is plotted as a function of $\ln(h/T^*)$ for the cases $U/\pi\Delta = 3, 5$. The two results are compared with the result $1/\cos^2(\pi m(h))$, where $m(h)$ is calculated from the Bethe ansatz results for the localized model where all impurity charge fluctuations are suppressed.

stance, for the temperature dependence of the susceptibility and magnetization we can use the thermodynamic relation,

$$\frac{\partial^2 C(T, H)}{\partial H^2} = T \frac{\partial^2 \chi(T, H)}{\partial T^2},$$  \hspace{1cm} (15)

where $C(T, H)$ is the specific heat. Applying this to the impurity contribution and taking the limit $T \to 0$ we find

$$\frac{\partial^2 \chi_s(T, H)}{\partial T^2} \bigg|_{T=0} = \frac{\partial^2 \gamma_d(H)}{\partial H^2}. \hspace{1cm} (16)$$

We can use the result in equation (16) to deduce the results for the $T^2$ dependence for $\chi_s(T, h)$,

$$\chi_s(0, h) - \chi_s(T, h) = -\frac{\pi^2}{12} \frac{T^2}{\chi_s(0, h)} \frac{\partial^2 \rho_d(0, h)}{\partial h^2} \hspace{1cm} (17)$$

On integrating these results with respect to $h$ we can derive a similar relation for the induced magnetization, $M(T, h) = m(T, h)/(g\mu_B)$,

$$m(0, h) - m(T, h) = -\frac{\pi^2}{6} T^2 \frac{\partial \rho_d(0, h)}{\partial h} = c_m(h) \left( \frac{T}{T^*} \right)^2. \hspace{1cm} (18)$$

We can calculate the coefficients $c_\chi(h)$ and $c_m(h)$ analytically in the non-interacting case,

$$c_\chi(0) = \frac{\pi^4}{48} \frac{(h/4T^*)^2}{\left[1 + (\pi h/4T^*)^2\right]^2}, \hspace{1cm} (19)$$

where $T^* = \Delta/4$.

We can also deduce the values of $c_\gamma(h)$ and $c_m(h)$ in the Kondo regime from the Bethe ansatz results for $\chi_d(0, H)$. As the Wilson or $\chi/\gamma$ ratio $R$ has the value 2 in this regime, independent $H$ as the charge fluctuations can be neglected, the value of $\gamma_d(H)$ can be deduced and is proportional to $\chi_d(0, H)$. On substituting the value for $\gamma_d(H)$ into equation (16), $c_\chi(h)$ and $c_m(h)$ can then be calculated. The asymptotic values as $h \to 0$ are $c_\chi(0) = \sqrt{3}\pi^3/8 + O(h^2)$ and $c_m(h) = h\sqrt{3}\pi^3/16T_K + O(h^3)$.

In figure 9 we plot the results for $-\tilde{\rho}_d(h)/\tilde{\rho}_d(0)$, which is proportional to $c_m(h)$, for $U/\pi\Delta = 3, 0, 0.5, 0.0$ in the range $0 < h/T^* < 2.5$. It can be seen that all three curves have a maximum which implies that $c_m(h)$ has a zero, and therefore changes sign from positive to negative in this range. In the non-interacting case it can be seen from the result in equation (18) that the change of sign occurs when $h/T^* = 4/\pi\sqrt{3}$, and from figure 9 that it occurs for $h$ significantly smaller than $T_K$ in the Kondo regime.

\section{V. LOW TEMPERATURE TRANSPORT IN AN ARBITRARY MAGNETIC FIELD}

To extend the calculations to the low energy dynamics we use the renormalized perturbation theory, which is described briefly in the Appendix. In this form of perturbation theory we work with the renormalized parameters, $\varepsilon_d$, $\Delta$ and $\tilde{U}$ instead of the original bare parameters $\varepsilon_d$, $U$,
\( \Delta \) and \( U \). The free propagators are those of the non-interacting quasiparticles and the expansion is in powers of \( \tilde{U} \). As the parameters are already fully renormalized counter terms have to be introduced to cancel any further renormalization. This expansion is completely specified by the three parameters \( \tilde{\varepsilon}_d, \Delta \) and \( U \), and is not restricted to the low energy regime, but valid for all energy scales. In practice, however, the calculations are easier to carry out in the low energy regime, where asymptotically exact results can be obtained in this regime by working only to second order in \( \tilde{U} \).

Here we exploit the fact that we have these renormalized parameters as a function of arbitrary magnetic field for the symmetric model to calculate the low energy dynamics in the presence of a magnetic field. The quasiparticle retarded Green function for the impurity level \( \tilde{G}_d(\omega, T, h) \) takes the form

\[
\tilde{G}_{d,\sigma}(\omega, T, h) = \frac{1}{\omega + \sigma \tilde{\varepsilon}_d(h) + i\Delta(h) - \tilde{\Sigma}_\sigma(\omega, T, h)},
\]

where \( \tilde{\Sigma}_\sigma(\omega, T, h) \) is the renormalized self-energy.

To calculate the leading order \( T^2 \) term in the transport coefficients we need \( \tilde{\Sigma}_\sigma(\omega, T) \) both to order \( \omega^2 \) and to order \( T^2 \). We calculate this from the renormalized perturbation expansion taken to order \( U^2(h) \). This takes full account of the quasiparticle scattering and gives the exact result of Yamada for \( h = 0 \). The corrections to order \( \omega^2 \) can be deduced from the second derivative of the self-energy with respect to \( \omega \) evaluated at \( \omega = 0 \) and \( T = 0 \). The result for the renormalized self-energy to this order is given by

\[
\tilde{\Sigma}_\sigma(\omega, 0, h) = -\tilde{\alpha}(h)\omega^2 \left[ i - (2 + \tilde{\alpha}(h))\sigma\tilde{\varepsilon}(h) \right],
\]

where \( \tilde{\varepsilon}(h) = \tilde{\varepsilon}_d(h)/\tilde{\Delta}(h) \), and \( \tilde{\alpha}(h) \) is given by

\[
\tilde{\alpha}(h) = \frac{\pi}{2}\tilde{\rho}_d(0, h)(R(h) - 1)^2,
\]

and \( \sigma_{\omega}(h) \) by

\[
\tilde{\sigma}_{\omega}(h) = \frac{2I(h)\tilde{\Delta}(h)}{\xi(h)c_0^2(0, h)},
\]

where \( \tilde{\xi}(h) = \pi\tilde{\rho}_d(0, h)\tilde{\Delta}(h)\tilde{\varepsilon}(h) \) and \( I(h) \) is the integral

\[
I(h) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{G}_d^0(\omega'')\tilde{G}_d^0(\omega'' + \omega')\tilde{G}_d^0(\omega')d\omega''d\omega'
\]

\( \tilde{G}_d^0(\omega) \) is the propagator in the diagrammatic expansion for \( T = 0 \) which is given by

\[
[\tilde{G}_d^0(\omega)]^{-1} = \omega + \sigma\tilde{\varepsilon}_d(h) + \text{sgn}(\omega)i\tilde{\Delta}(h).
\]

The corresponding result for the renormalized self-energy to order \( T^2 \) can be derived using the Sommerfeld expansion. The calculation can be performed by using for each internal propagator \( \tilde{G}_d^0(\omega) \) in the \( T = 0 \) diagrammatic expansion an additional correction term,

\[
-\frac{(\pi T)^2}{3} \frac{\delta'(\omega)\tilde{\Delta}(h)}{(\omega + \sigma\tilde{\varepsilon}_d(h))^2 + \Delta^2(h)}.
\]

The result for the renormalized self-energy to order \( T^2 \) for \( \omega = 0 \) is

\[
\tilde{\Sigma}_\sigma(T, 0, h) = -\tilde{\alpha}(h)(\pi T)^2 \left[ i + \sigma\tilde{\varepsilon}(h)(1 + \tilde{\alpha}_{T}(h)) \right],
\]

where the parameter \( \tilde{\alpha}_{T}(h) \) is given by

\[
\tilde{\alpha}_{T}(h) = \frac{1}{6\xi(h)\tilde{\varepsilon}(h)} \left[ 1 - \tilde{\varepsilon}(h)\tan^{-1}(\tilde{\varepsilon}(h)) \right].
\]

We can now apply these results to the calculation of transport coefficients.

### A. Application to magnetic impurities

The contribution to the conductivity from the scattering of isolated impurities described by an AIM, \( \sigma(T, h) \), given by

\[
\sigma(T, h) = \sigma_0 \sum_\sigma \int_{-\infty}^{\infty} \frac{1}{\rho_{d,\sigma}(\omega, T, h)} \left( -\frac{\partial f(\omega)}{\partial \omega} \right) d\omega,
\]

where \( \rho_{d}(\omega, T, h) = \tilde{\Delta}(h)\tilde{\rho}_{d}(\omega, T, h)/\Delta \), and \( \tilde{\rho}_{d}(\omega, T, h) \) is the spectral density of the quasiparticle Green function \( \tilde{G}_d(\omega, T, h) \). The Sommerfeld expansion gives for \( \sigma_0 \) to second order in \( T \),

\[
\sigma(T, h) = \sigma_0 \left\{ \sum_\sigma \left[ \frac{1}{\rho_{d,\sigma}(0, T, h)} + \left[ \sum_\sigma \left( \frac{\rho_{d,\sigma}(0, h)^2}{\rho_{d,\sigma}(0, h)} - \frac{\rho_{d,\sigma}(0, 0, h)}{\rho_{d,\sigma}(0, 0, h)} \right) \right] \frac{(\pi T)^2}{6} \right\},
\]

where the prime refers to a derivative with respect to \( \omega \). Note that the first term still contains a temperature dependence via \( \rho_{d} \).

On using the renormalized self-energy to calculate the quasiparticle spectral density \( \tilde{\rho}(\omega, T, h) \), and substituting in equation (30), the final result for \( \sigma(T, h) \) to order \( T^2 \) is

\[
\sigma(h, T) = \sigma(h, 0) \left\{ 1 + \sigma_2(h) \left( \frac{\pi T}{\Delta(h)} \right)^2 + O(T^4) \right\},
\]

where \( \sigma(h, 0) = 2\sigma_0/\cos^2(\pi m(h)) \) and \( \sigma_2(h) \) is given by

\[
\sigma_2(h) = \frac{\cos^2(\pi m(h))}{3} \left[ 1 + C(h)(R(h) - 1)^2 \right].
\]

The coefficient \( C(h) \) is

\[
C(h) = \cos^2(\pi m(h)) - \sin^2(\pi m(h)) \left[ 1 - 3\tilde{\alpha}(h) + \tilde{\alpha}_{\omega}(h) \right].
\]
the conductivity. Weak coupling \((32)\) for the second order temperature expansion of the conductivity. Weak coupling \((U/\pi \Delta = 0.5)\) up to strong coupling \((U/\pi \Delta = 4)\) is considered.

In figure 10 we show the second order coefficient \(\sigma_2(h)\) plotted over \(\log(h/T^*)\) for a range of parameters \((U/\pi \Delta = 0.5 - 4)\). For zero field the conductivity rises with temperature as is well known.5 When \(h\) is increased \(\sigma_2(h)\) decreases and tends to zero for very high fields, so that the low temperature conductivity becomes temperature independent. The impurity level is then shifted out of the range of the thermally excited states in the conduction band so that there is negligible impurity scattering. We note for the strong coupling cases where there is a local moment \((U/\pi \Delta = 2, 4)\), the coefficient \(\sigma_2(h)\) changes sign for a certain critical field \(h_c\), with \(h_c \sim 0.5 T^*\). This does not arise, as one could expect from the change of the impurity density of states at the Fermi level with the field \[\text{second term in (30)}\], but from the temperature dependence of the self-energy, which contributes in the first term in \(\text{[30]}\). To see this only consider the imaginary part contribution to the self-energy, \[\text{[27]}\] which leads to a \(T^2\) term

\[(\pi T)^2/2(R(h) - 1)^2[\cos^2(\pi m(h)) - \sin^2(\pi m(h))].\quad (34)\]

This expression clearly changes sign when \(m(h)\) exceeds \(1/4\) or \(\tilde{\varepsilon}_d(h) > \tilde{\Delta}(h)\). In contrast the contribution from the second term in \(\text{[30]}\) with only the imaginary part of the self-energy taken into account gives

\[(\pi T)^2/3(1 + (R(h) - 1)^2[\cos^2(\pi m(h)) - \sin^2(\pi m(h))]\]. \quad (35)\]

which cannot change sign. Including the real part contribution does not alter this behaviour substantially.

Physically, it is the spin flip scattering of the local moment that causes the resistance to rise as the temperature is lowered, leading to a resistance minimum and the Kondo effect. Perturbation theory shows that spin-flip scattering gives a diverging amplitude for \(T \simeq T^*\). For a mainly polarized impurity spin these processes are, however, strongly suppressed, and the change in sign of the temperature dependence might be attributed to the thermal spin disorder scattering. To our knowledge, this effect has not been observed but for magnetic impurities systems with a very low Kondo temperature it might be feasible to put the result to an experimental test.

B. Application to quantum dots

The Kondo effect in a magnetic field has been observed experimentally in mesoscopic systems, for example, quantum dots in heterostructures.23 Such systems can be quantitatively described by the Anderson impurity model19,20. The symmetric Anderson model corresponds to the situation, where the gate voltage \(V_g\) is tuned to the middle of a Coulomb valley with odd number of electrons on the dot.

Hershfield et al.22 and Meir and Wingreen26 derived an expression for the current through a quantum dot by a non-equilibrium calculation, which for the case of symmetric coupling to the leads takes the form

\[ I = \frac{G_0\Delta}{2e} \sum_\sigma \int d\omega \left(-\text{Im} G_{ds}^{\text{noneq}}(\omega)\right) \times \left[n_F(\omega - \mu_L) - n_F(\omega - \mu_R)\right], \quad (36)\]

where \(n_F\) is the Fermi function, \(G_{ds}^{\text{noneq}}\) is the retarded non-equilibrium Green function from the Keldysh formalism on the dot, \(\mu_L = \mu + eV/2, \mu_R = \mu - eV/2\) are the chemical potentials in left, right lead, respectively, and \(V = V_{ds}\) the source drain voltage.22 \(G_0 = e^2/\pi \hbar\) with Planck’s constant \(\hbar\).

In the limit of linear response the equilibrium value of the one-electron Green function can be used to evaluate \[\text{[30]}\], and the resulting expression for the differential conductance \(G = dI/dV\) through a quantum dot is

\[ G(T, h) = \frac{G_0\Delta}{2} \sum_\sigma \int d\omega \pi \rho_d,\sigma(\omega, T, h) \left(-\frac{\partial n_F(\omega)}{\partial \omega}\right). \quad (37)\]

In the low temperature regime we can again apply the Sommerfeld expansion to obtain the leading order finite...
temperature corrections to order $T^2$, 

$$G(T, h) = \frac{G_0 \Delta}{2} \left[ \sum_\sigma \pi \rho_{d, \sigma}(0, T, h) + \left( \sum_\sigma \pi \rho_{d, \sigma}''(0, 0, h) \right) \left( \frac{\pi T}{6} \right)^2 \right].$$

(38)

Here, in contrast to the earlier case the second term changes sign for a critical field $h_c$ when $\sum_\sigma \rho_{d, \sigma}(\omega, 0, h)$ changes from a maximum to a local minimum at $\omega = 0$. For free quasiparticles this happens when $\tilde{\varepsilon}_d(h_c) = \tilde{\Delta}(h_c)/\sqrt{3}$, as discussed in detail in reference 24. The temperature dependent part of the first term in equation (38) including only the imaginary part from the self-energy is

$$\frac{1}{2\Delta} (R(h) - 1)^2 \frac{\sin^2(\pi \rho_m(h)) - \cos^2(\pi \rho_m(h))}{(1 + \tan^2(\pi \rho_m(h)))^2},$$

(39)

and this also changes sign for $m(h) > 1/4$. The total result is

$$G(T, h) = G(0, h) \left[ 1 - G_2(h) \left( \frac{\pi T}{\Delta(h)} \right)^2 \right],$$

(40)

with

$$G(0, h) = G_0 \cos^2(\pi \rho_m(h)),$$

(41)

and

$$G_2(h) = \frac{\cos^2(\pi \rho_m(h))}{3} \left\{ \cos^2(\pi \rho_m(h)) \left[ 1 + 2(R(h) - 1)^2 \right] \right.$$

$$- \sin^2(\pi \rho_m(h)) \left[ 3 + (R(h) - 1)^2(1 + 2\alpha_\omega(h) - 6\alpha_T(h)) \right] \right\}.$$

In figure 11 the field dependence of $G_2(h)$ is shown. Note that we have included a minus sign before the $T^2$ term in (40), so that the similar behaviour in figures 10 and 11 actually corresponds to opposite temperature dependence. This is due to the approximate inverse relation between the two systems, if the hybridization $V_h = 0$ for an impurity, there is no scattering and hence infinite conductivity, whereas if $V_h = 0$ for the quantum dot there is no current and hence infinite resistivity.

VI. BEYOND THE LOW ENERGY REGIME

We can use the extension of the NRG method to the calculation of dynamic response functions to look at the behaviour of the model in an arbitrary magnetic field on higher energy scales. In doing so it is important to use the density matrix (DM-NRG) method introduced by Hofstetter as the standard NRG approach gives results which considerably underestimate the shift of the high energy spectral weight with the variation of magnetic field. We also use the approach of Bulla et al. in which the self-energy is deduced from the calculation of higher order Green functions, as this gives more accurate results. In figure 12 we give results for the spin up part of the d-site spectral density $\rho_{d, \uparrow}(\omega) = -\frac{1}{\pi} \text{Im} G_{d, \uparrow}(\omega^+) / \text{Im} G_{d, \uparrow}(\omega^+)$ for a strong coupling situation ($U/\pi \Delta = 4$) for various values of the magnetic field $h$. The shift of the spin-up Kondo resonance from the Fermi level with increase of magnetic field, which is almost imperceptible on the scale shown, is accompanied by large shifts of the spectral weight on the higher energy scales as the impurity is magnetically polarized.

In order to test the improved estimates of this shift from the DM-NRG, we calculate $\langle n_\uparrow \rangle$ by integrating the spectral density up to the Fermi level to deduce the value of the induced magnetization $m$. This result can then be compared with that calculated earlier from the renormalized parameters using equation (9), and also with the values calculated directly from the ground state occupation numbers at the impurity site, as deduced from the matrix elements in the NRG routine. The results are shown in figure 13 for the three parameter regimes $U/\pi \Delta = 0.5, 1, 4$ over $\ln(h/\pi \Delta)$. The magnetization departs from zero already for very low $h/\pi \Delta$ in the strong coupling case due to the induced lower energy scale $\Delta$, 

FIG. 11: Field dependent coefficient $G_2(h)$ for the second order temperature expansion of the conductance. Weak coupling ($U/\pi \Delta = 0.5$) up to strong coupling ($U/\pi \Delta = 4$) is considered.
whereas for the intermediate and weak coupling cases higher fields are required to show similar behaviour. For large $h$ all three merge and approach a saturation value $m_s = \frac{1}{2}$, corresponding to complete polarization of the electron on the impurity site. The agreement of the results is excellent in the three parameter regimes for all $h$, and confirms that the spectral weight in a broken symmetry situation can be computed correctly using the DM-NRG.

In figure 14, we focus on the shift of the quasiparticle (Kondo) resonance in the results for the strong coupling case ($U/\pi \Delta = 4$) as in figure 12. This shift of the resonance from the Fermi level ($\omega = 0$) with increasing magnetic field values is clearly seen on the higher resolution energy scale used for this plot. As the peak shifts, its height decreases and the resonance becomes broader. For even larger fields than shown here the peak merges with the lower atomic limit peak seen in figure 12. Note that the peak form is asymmetric with logarithmic tails, similar to the results of Rosch et al., obtained using the perturbative RG for the Kondo model. However, some of the asymmetry in the our results must be attributed to the logarithmic broadening scheme.

If $-\varepsilon_p(h)$ is the position of the quasiparticle peak in the spectral density for a spin up electron, then the corresponding value for non-interacting electrons ($U = 0$) is half the Zeeman splitting, $\Delta Z$, where $\Delta Z = 2h$. An exact expression for $\varepsilon_p(h)/h$ in the limit $h \to 0$ has been derived by Logan and Dickens, written as

$$\lim_{h \to 0} \frac{\varepsilon_p(h)}{h} = \frac{R}{1 + b\Delta Z^2}.$$  \hspace{1cm} (42)

This ratio, therefore, varies from 1 in the non-interacting case ($R = 1$) to 4/3 in the Kondo limit ($R = 2$). It is not straight forward to obtain a precise estimate of $b$ or the value of $\varepsilon_p(h)$ from the DM-NRG spectra as they are sensitive to parameters of the logarithmic scale Gaussian broadening which is used to obtain a continuous spectrum on all energy scales from the discrete results. However, if the broadening is modified to Lorentzian peaks with constant width for the very low energy scales the asymptotic results can be confirmed.
We have estimated the ratio $\varepsilon_p(h)/h$ from the NRG spectra for higher magnetic field values and find that the it increases monotonically with $h$ and exceeds the value of 2 before the peak merges at high field values into the atomic-like peaks. There have been other estimates of the $h$-dependence of this ratio\textsuperscript{20,31,32}, but these differ markedly according to the method of calculation. On the basis of a Bethe ansatz calculation of the spinon spectrum for the Kondo model Moore and Wen\textsuperscript{1} find that $\varepsilon_p(h)/h < 2$ in all cases and conjecture that the value of 2 is the high field asymptotic limit. It is possible that this is a feature of the localized model, when charge fluctuations are completely suppressed. There is some evidence in support of this in our results in that, as we suppress the charge fluctuations on increasing the value of $U$ through the values $U/\pi\Delta = 2, 3, 4$, the ratio $\varepsilon_p(h)/h$ increases less rapidly with increase of $h$. The ratio only begin to exceed the value of 2 roughly at the point when charge fluctuations set in and $R(h)$ begins to differ significantly from the value of $R(h)$ for the localized model, $R(h) = 2$. Costi\textsuperscript{32} has also done NRG calculations for a localized model and finds a ratio close to but always less than 2. Using the local moment approximation Dickens and Logan\textsuperscript{33} have also estimated the ratio $\varepsilon_p(h)/h$ and find an even more marked increase in the ratio with increase of $h$ to values such that $\varepsilon_p(h)/h > 2$.

For all the curves one finds $a = 0.26 \pm 0.01$ independent of $h$. For the total spectral density, which we denote by $\rho_\delta(\omega)$, we need to include the contribution from the down spin, which has its peak at $\varepsilon_p(h)$, $\rho_\delta = \rho_{\delta,\uparrow} + \rho_{\delta,\downarrow}$. The splitting between the up and down peaks in the total spectrum is then $2\varepsilon_p(h)f_\uparrow(h)$, where $f_\uparrow(h)$ is a correction factor due to the overlap of the resonances\textsuperscript{24} In general it has to be determined numerically, but for free quasiparticles (see equation (20) without $\Sigma$) it is given by

$$f_\uparrow(h)^2 = 1 - \left(1 + \left(\Delta(h)/\varepsilon_\delta(h)\right)^2\right)^{1/2}.$$  

For higher fields one has $f_\uparrow(h) \approx 1 - \Delta^4/(8\varepsilon_\delta)^4$. In figure 15 we give an example for the total spectral density for the earlier used parameters $U/\pi\Delta = 4$ and a range of magnetic fields. Clearly, the peak splits above a critical field, $h \gtrsim 0.5T^\ast$, which is in agreement with results of Costi for the Kondo model\textsuperscript{32}.

**Comparison with experiments on quantum dots**

In section V.B we have calculated the lowest order temperature dependence of the conductance through a quantum dot in a magnetic field, $\rho_\delta(\omega)$, This temperature dependence has been observed in the zero magnetic field case\textsuperscript{20}. We noted earlier that there is a sign change in this leading temperature dependence at a values of the magnetic field $0 < h < T^\ast$. The sign change in the second term in equation (57) occurs when $\rho_\delta$ changes from a...
local maximum to a minimum as can be seen in figure 10. A qualitative explanation of this sign change is that the local spectral density of states at the Fermi level is suppressed with increasing magnetic field. At higher fields when the spectral density develops two peaks then there are more thermally excited states which can contribute to an increase of the conductance. This temperature dependence might be experimentally observable, since estimates of the Kondo temperature are of the order 300 mK corresponding to magnetic fields in the experimental range. A difficulty might be that the overall response is reduced because it serves as a local model of strong correlation.

We have calculated the non-equilibrium Green function by the equilibrium one. Hewson, Bauer and Ogiuri have calculated the non-equilibrium Green function for a small but finite voltage \( V \), and find that a finite voltage reduces the peak position substantially. We conclude that an accurate agreement of experiment and theory rests therefore on an accurate description of the steady state situation out of equilibrium. We are currently working on an extension of renormalized perturbation theory in the non-equilibrium formalism, which takes this situation into account appropriately.

VII. SUMMARY

We have shown that in an arbitrary magnetic field \( H \) it is possible to describe the quasiparticles of a Fermi liquid regime by field dependent parameters. We have used the particle-hole symmetric Anderson model as an illustration because of its wide range of applications and because it serves as a local model of strong correlation physics. For this model the three relevant field dependent parameters are the renormalized impurity levels with spin \( \sigma \), \( \tilde{E}_{\sigma}(H) \), the quasiparticle resonance width, \( \tilde{\Delta}(H) \) and the local interaction \( \tilde{U}(H) \). We have shown how these can be deduced from NRG calculations of the low lying excitations. Once the renormalized parameters are known, the impurity spin and charge susceptibility, the specific heat coefficient and the induced impurity magnetization can be obtained in a similar way. We have also extended the renormalized perturbation expansion in order to calculate the leading temperature dependence for the finite conductivity due to scattering from an impurity in a metallic host, and for the conductance through a quantum dot.

By choosing the bare parameters in the absence of the field to correspond to the strongly correlated or Kondo limit, the de-renormalization of the quasiparticles can be followed as the magnetic field strength is increased from zero. For extremely large magnetic fields the parameters revert to their bare values. This approach gives an overview of the low energy behaviour of the model as a function of the applied magnetic field strength.

A number of physical properties are found to change qualitatively in the strongly correlated case for magnetic field strengths in the range \( 0 < g \mu_B H < T_K \), where \( T_K \) is the Kondo temperature. This should be a physically measurable phenomenon.
accessible magnetic field range for many systems. The \(T^2\) coefficient of the magnetic susceptibility, the conductivity from a magnetic impurity in the strong correlation regime, and the conductance through a quantum dot all change sign in this magnetic field range.

The approach developed here is a general one and is equally applicable to asymmetric impurity models and to lattice models. For lattice models, for which dynamical mean field theory is applicable, similar NRG methods to those employed here can be used\(^{36}\), and our calculations are currently being extended to models of heavy fermions. We note that the approach is not restricted to the NRG method, the relevant renormalized parameters could also be estimated using other theoretical techniques, variational methods for example.

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VIII. APPENDIX: THE RENORMALIZED PERTURBATION APPROACH

We give a brief synopsis of the renormalized perturbation approach. This approach is best developed in the field theoretical Lagrangian formalism where the renormalization of the field is a more natural concept. The Lagrangian corresponding to the bare Anderson Lagrangian \(\mathcal{L}_{AW}(\varepsilon_d, \Delta, U)\) can be rewritten in the form
\[
\mathcal{L}_{AW}(\tilde{\varepsilon}_d, \tilde{\Delta}, \tilde{U}) = \mathcal{L}_{AW}(\varepsilon_d, \Delta, U) + \mathcal{L}_{ct}(\lambda_1, \lambda_2, \lambda_3),
\]
where the renormalized parameters, \(\tilde{\varepsilon}_d, \tilde{\Delta}\), are defined in terms of the self-energy \(\Sigma_\sigma(\omega)\) of the one-electron Green function for the impurity state,
\[
G_{d, \sigma}(\omega) = \frac{1}{\omega - \varepsilon_{d, \sigma} + i\Delta - \Sigma_\sigma(\omega)},
\]
and are given by
\[
\tilde{\varepsilon}_{d, \sigma} = \varepsilon_{d, \sigma} + \Sigma_\sigma(0), \quad \tilde{\Delta} = \Delta - \Sigma_\sigma(0),
\]
where \(\varepsilon_{d, \sigma}\) is given by \(\varepsilon_{d, \sigma} = 1/(1 - \Sigma_\sigma(0))\). The renormalized or quasiparticle interaction \(\tilde{U}\), is defined in terms of the local irreducible 4-vertex \(\Gamma_{\uparrow\downarrow}(\omega_1, \omega_2, \omega_3, \omega_4)\) at zero frequency,
\[
\tilde{U} = z_\uparrow z_\downarrow \Gamma_{\uparrow\downarrow}(0, 0, 0, 0).
\]

The remaining part of the Lagrangian \(\mathcal{L}_{ct}(\lambda_1, \lambda_2, \lambda_3)\) contains three counter terms with coefficients \(\lambda_1, \lambda_2\) and \(\lambda_3\). A perturbation expansion in powers of the quasiparticle interaction \(\tilde{U}\) can then be carried out provided the counter terms are also taken into account. The counter terms \(\lambda_1, \lambda_2\) and \(\lambda_3\) are determined to each order in \(\tilde{U}\) by the renormalization conditions\(^{36}\),
\[
\tilde{\Sigma}_\sigma(0) = 0, \quad \tilde{\Sigma}_\sigma'(0) = 0, \quad \tilde{\Gamma}_{\uparrow\downarrow}(0, 0, 0, 0) = \tilde{U}
\]
where \(\tilde{\Sigma}(\omega)\) and \(\tilde{\Gamma}_{\uparrow\downarrow}(\omega_1, \omega_2, \omega_3, \omega_4)\) are the renormalized self-energy and irreducible 4-vertex, respectively.

The renormalized parameters, as defined in equations \(^{49}\) and \(^{50}\), can be calculated in low order perturbation theory\(^2\), but these calculations cannot be extended to the more physically interesting strong coupling regime \(U/\pi\Delta > 2\). These parameters, however, can be identified with those in equation \(^{48}\), and so they can alternatively be deduced from the levels in the numerical renormalization group calculations, which can be carried out for all values of \(U\). The expressions given earlier for the impurity occupation number at \(T = 0\), the specific heat coefficient and spin and charge susceptibilities, \(^{35}\) and \(^{36}\), are exact and correspond to first order calculations in a renormalized perturbation expansion\(^6\) in powers of \(\tilde{U}\). Calculations carried out to second order in \(\tilde{U}\) give exact results for the leading low order temperature dependence to the impurity resistivity\(^6\), and the leading non-linear term in the differential conductivity\(^37,38\).
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