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Renormalized perturbation calculations for the single-impurity Anderson model

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Abstract
We illustrate the renormalized perturbation expansion method by applying it to a single-impurity Anderson model. Previously, we have shown that this approach gives the *exact* leading-order results for the specific heat, spin and charge susceptibilities and leading-order temperature dependence of the resistivity for this model in the Fermi-liquid regime, when carried out to second order in the renormalized interaction $\tilde{U}$. Here we consider the effects of higher-order quasiparticle scattering and calculate the third-order contributions to the H^3-term in the impurity magnetization for the symmetric model in a weak magnetic field H. The result is asymptotically exact in the weak-coupling regime, and is very close to the exact Bethe *ansatz* result in the Kondo regime. We also calculate the quasiparticle density of states in a magnetic field, which is of interest in relation to recent experimental work on quantum dots.

1. Introduction

Systems with strong local inter-electron interactions have been the focus of much theoretical work in recent years, as these include a variety of interesting systems ranging from high-T_c superconductors, heavy fermions and Mott insulators, to mesoscopic systems such as quantum dots. Conventional perturbation theory cannot deal with strong interactions in general, so new techniques have to be developed to make predictions for the behaviour of such systems. Specialized techniques, such as the Bethe *ansatz* or conformal field theory, have been successfully developed for certain classes of systems, such as one-dimensional systems and impurity models. However, techniques are required that can be applied more generally, particularly for systems in two and three dimensions. One approach which has been extended to a wider class of problems is the numerical renormalization group approach (NRG) as developed by Wilson [1], which was originally successfully applied to models of magnetic impurities. In this approach the higher-energy excitations are progressively eliminated to deduce a sequence of effective models for the behaviour on lower and lower energy scales. The behaviour on the lowest energy scales can be calculated from the limiting fixed-point Hamiltonian of this sequence, and its leading correction terms. In its original form the method only works for impurity systems but a modified form of the approach, the density matrix renormalization group method (DMRG) [2,3], has been successfully developed for one-dimensional systems. In principle the DMRG could be extended to two and three dimensions but there are technical difficulties in practice, though some calculations for two-dimensional systems have been carried out. In another development the NRG has also been extended to higher-dimensional lattice models by use of dynamical mean-field theory (DMFT) [4]. This approach exploits the fact that certain infinite-dimensional lattice models, such as the Hubbard and periodic Anderson models, can mapped onto effective impurity models, together with a self-consistency condition [5, 6]. The calculations for the effective impurity models can be carried out using the NRG and iterated until the self-consistency condition is satisfied. The DMFT has considerably extended the potential range of application of the NRG. The NRG, however, is not the only way of realizing renormalization group ideas. The earlier way of applying the renormalization group, as originally developed in field theory, was via a reorganization of the perturbation expansion, such that the expansion could be carried out in terms of the renormalized parameters. This rearrangement of perturbation theory enabled one to circumvent the problem of the divergences which had plagued the conventional approaches. The elimination of the divergences, however, was essentially a by-product of this approach and it is possible to use the reorganization of the perturbation expansion as a strategy for dealing with the low-energy behaviour of a wide variety of systems. The renormalized perturbation theory approach could be particularly useful in situations where there are strong renormalizations of the basic parameters, such as in the Fermi-liquid regime for heavy fermions, where the masses of the electrons may be renormalized by factors of the order of 1000.

In earlier work [7] we have shown how the renormalized perturbation theory can be applied to impurity models. In particular, we have shown that this approach, when applied to the Anderson impurity model and carried out to second order in the renormalized interaction $\tilde{U}$, gives the exact leading-order results for the specific heat, spin and charge susceptibilities at $T = 0$ and the leading-order temperature dependence of the resistivity in the Fermi-liquid regime. In this paper we begin with a brief review of these earlier results, and we then calculate some higher-order corrections; in particular, we calculate the H^3-term for the impurity magnetization in a weak magnetic field H to third order in the renormalized interaction term $\tilde{U}$, and compare the results with the exact Bethe *ansatz* result. In the final section we calculate the quasiparticle density of states in a magnetic field. These latter results are of some interest in comparing with the low-temperature linear response results on quantum dots in the presence of a magnetic field.

2. Renormalized perturbation theory

We formulate the renormalized perturbation expansion for the impurity Anderson model [8]. The Hamiltonian for this model is

$$H = \sum_{\sigma} \epsilon_{\rm d} d^{\dagger}_{\sigma} d_{\sigma} + U n_{{\rm d},\uparrow} n_{{\rm d},\downarrow} + \sum_{k,\sigma} (V_k d^{\dagger}_{\sigma} c_{k,\sigma} + V^{*}_{k} c^{\dagger}_{k,\sigma} d_{\sigma}) + \sum_{k,\sigma} \epsilon_{k,\sigma} c^{\dagger}_{k,\sigma} c_{k,\sigma} \tag{1}$$

which describes an impurity d level $\epsilon_{\rm d}$, hybridized with conduction electrons of the host metal via a matrix element V_k, with a term U describing the interaction between the electrons in the localized d state, where $n_{{\rm d},\sigma} = d^{\dagger}_{\sigma} d_{\sigma}$. The width of the localized bound state for $U = 0$ depends on the quantity $\Delta(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k)$. For a conduction without any prominent features this function does not have a strong dependence on ω, so it is usual to take the case of a wide conduction band with a flat density of states where $\Delta(\omega)$ becomes independent of ω and can be taken as a constant, Δ. The partition function Z for this model can be expressed as a functional integral over imaginary time-dependent Grassmann variables, corresponding to the electron creation and annihilation operators, using standard methods (see for example [9]):

$$Z = \int \prod_{\sigma} \mathcal{D}(\bar{d}_\sigma)\,\mathcal{D}(d_\sigma)\,\mathcal{D}(\bar{c}_{k,\sigma})\,\mathcal{D}(c_{k,\sigma})\,\mathrm{e}^{-S} \tag{2}$$

where the action S is given by

$$S = \int_0^\beta \mathcal{L}_{\mathrm{AM}}(\tau)\,\mathrm{d}\tau \tag{3}$$

and the Lagrangian for the Anderson model is given by

$$\mathcal{L}_{\mathrm{AM}}(\tau) = \sum_\sigma \bar{d}_\sigma(\tau)(\partial_\tau - \epsilon_{\mathrm{d}})d_\sigma(\tau) + \sum_{k,\sigma} \bar{c}_{k,\sigma}(\tau)(\partial_\tau - \epsilon_k)c_{k,\sigma}(\tau) + Un_\uparrow(\tau)n_\downarrow(\tau) + \sum_\sigma V_k(\bar{d}_\sigma(\tau)c_{k,\sigma}(\tau) + \bar{c}_{k,\sigma}(\tau)d_\sigma(\tau)) \tag{4}$$

where $n_\sigma(\tau) = \bar{d}_\sigma(\tau)d_\sigma(\tau)$. One can formally integrate over the Grassmann variables for the conduction electrons, as they involve only quadratic terms, and express the result in terms of a reduced action S_{red}:

$$Z = \int \prod_\sigma \mathcal{D}(\bar{d}_\sigma)\,\mathcal{D}(d_\sigma)\,\mathrm{e}^{-S_{\mathrm{red}}} \tag{5}$$

where S_{red} is given by

$$S_{\mathrm{red}} = \int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' \sum_\sigma \bar{d}_\sigma(\tau)[G_\sigma^{(0)}(\tau - \tau')]^{-1} d_\sigma(\tau') + U \int_0^\beta \mathrm{d}\tau\, n_\uparrow(\tau)n_\downarrow(\tau) \tag{6}$$

with $G_\sigma^{(0)}(\tau) = (1/\beta)\sum_n G_\sigma^{(0)}(\mathrm{i}\omega_n)\mathrm{e}^{-\mathrm{i}\omega_n\tau}$, where $\omega_n = (2n+1)\pi/\beta$. The non-interacting Green's function for the localized electron $G_\sigma^{(0)}(\mathrm{i}\omega_n)$ is given by

$$G_\sigma^{(0)}(\mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n + \sigma h - \epsilon_{\mathrm{d}} + \mathrm{i}\Delta\,\mathrm{sgn}(\omega_n)} \tag{7}$$

where we have included a coupling to a magnetic field H and h is given by $h = g\mu_{\mathrm{B}}H/2$. The Grassmann variables are required to satisfy the antiperiodic boundary conditions $\bar{d}(\beta) = -\bar{d}(0)$ and $d(\beta) = -d(0)$.

The Fourier transform of the corresponding retarded one-particle double-time Green's function $G_{\mathrm{d}\sigma}^{(0)}(\omega)$ for the localized d electron can be deduced by analytically continuing to real frequencies, $\mathrm{i}\omega_n \to \omega + \mathrm{i}\delta$ ($\delta \to +0$). On introducing a corresponding self-energy $\Sigma_\sigma(\omega, h)$ the interacting retarded Green's function can be written in the form

$$G_\sigma(\omega) = \frac{1}{\omega - \epsilon_{\mathrm{d}} + \sigma h + \mathrm{i}\Delta - \Sigma_\sigma(\omega, h)}. \tag{8}$$

In the conventional perturbation expansion this self-energy is calculated in powers of the interaction U. It will be convenient to write the self-energy in the form $\Sigma_\sigma(\omega+\sigma h, h)$ because the non-interacting Green's functions, which are the propagators in the perturbation expansion, are functions of the combined variable $\omega + \sigma h$. In the renormalized perturbation theory the perturbation expansion is reorganized to a form appropriate for the low-energy regime. The first step is to write the self-energy in the form

$$\Sigma_\sigma(\omega + \sigma h, h) = \Sigma_\sigma(0, 0) + (\omega + \sigma h)\Sigma'_\sigma(0, 0) + \Sigma_\sigma^{\mathrm{rem}}(\omega, h) \tag{9}$$

which does nothing more than define the remainder self-energy $\Sigma_\sigma^{\mathrm{rem}}(\omega + \sigma h, h)$, except that we have assumed Luttinger's result [11] that $\Sigma'_\sigma(0, 0)$ is real. When this is substituted back into equation (8), the Green's function takes the same form with a 'renormalized' energy level, width of the localized state and self-energy, which are denoted by a tilde, defined by

$$\tilde{\epsilon}_{\rm d} = z(\epsilon_{\rm d} + \Sigma_\sigma(0,0)) \qquad \tilde{\Delta} = z\Delta \qquad \tilde{\Sigma}_\sigma(\omega,h) = z\Sigma_\sigma^{\rm rem}(\omega,h) \tag{10}$$

where z, the wavefunction renormalization factor, is given by $z = 1/(1 - \Sigma'_\sigma(0,0))$, and $\Sigma_\sigma(0,0)$ and $\Sigma'_\sigma(0,0)$ are to be evaluated at $T = 0$ as well as $\omega = h = 0$. These will be the parameters of the renormalized theory instead of $\epsilon_{\rm d}$ and Δ, which are specified in the 'bare' Hamiltonian of equation (1). Note that the g-factor coupling to the magnetic field H is unrenormalized. The overall z-factor is removed by rescaling the Grassmann fields, $d_\sigma(\tau) \to \sqrt{z}\tilde{d}_\sigma(\tau)$.

The last parameter specifying the renormalized theory is the renormalized interaction $\tilde{U}$. This quantity is derived from the irreducible four-point vertex function ('four-vertex') $\Gamma_{\sigma,\sigma'}(\omega,\omega')$, which is a special case of the more general irreducible four-point vertex function $\Gamma_{\sigma,\sigma'}^{\sigma'',\sigma'''}(\omega,\omega';\omega'',\omega''')$ with $\sigma'' = \sigma$, $\sigma''' = \sigma'$, $\omega'' = \omega$ and $\omega''' = \omega'$. This latter quantity is derived from the two-particle Green's function of the d electrons in the usual way. The renormalized four-point vertex function is defined by $\tilde{\Gamma}_{\sigma,\sigma'}(\omega,\omega') = z^2\Gamma_{\sigma,\sigma'}(\omega,\omega')$, and takes account of the rescaling of the local fermion fields. The renormalized interaction $\tilde{U}$ is then defined by the value of $\tilde{\Gamma}_{\sigma,\sigma'}(\omega,\omega')$ at $\omega = \omega' = 0$:

$$\tilde{U} = \tilde{\Gamma}_{\sigma,\sigma'}(0,0). \tag{11}$$

As certain of the interaction effects are taken into account *ab initio* in the renormalized theory, compensating terms have to be introduced to avoid overcounting. The Lagrangian for the Anderson model can be rewritten in the form

$$\mathcal{L}_{\rm AM}(\bar{d}_\sigma, d_\sigma, \epsilon_{\rm d}, \Delta, U) = \mathcal{L}_{\rm AM}(\tilde{\bar{d}}_\sigma, \tilde{d}_\sigma, \tilde{\epsilon}_{\rm d}, \tilde{\Delta}, \tilde{U}) + \mathcal{L}_{\rm CT}(\tilde{\bar{d}}_\sigma, \tilde{d}_\sigma, \lambda_1, \lambda_2, \lambda_3) \tag{12}$$

in terms of the renormalized fields, where the counter-term Lagrangian is given by

$$\mathcal{L}_{\rm CT}(\tilde{\bar{d}}_\sigma, \tilde{d}_\sigma, \lambda_1, \lambda_2, \lambda_3) = \tilde{\bar{d}}_\sigma(\tau)(\lambda_2\,\partial_\tau + \lambda_1)\tilde{d}_\sigma + \lambda_3\tilde{n}_\uparrow(\tau)\tilde{n}_\downarrow(\tau) \tag{13}$$

where $\lambda_1 = -z\Sigma(0,0)$, $\lambda_2 = z - 1$ and $\lambda_3 = z^2(U - \Gamma_{\uparrow,\downarrow}(0,0))$. By construction, the renormalized self-energy $\tilde{\Sigma}_\sigma(\omega,0)$ is such that

$$\tilde{\Sigma}_\sigma(0,0) = 0 \qquad \tilde{\Sigma}'_\sigma(0,0) = 0 \tag{14}$$

so $\tilde{\Sigma}_\sigma(\omega,0) = {\rm O}(\omega^2)$ for small ω, on the assumption that it is analytic at $\omega = 0$. As $\tilde{\Gamma}_{\sigma,\sigma}(0,0) = 0$, we also have

$$\tilde{\Gamma}_{\sigma,\sigma'}(0,0) = \tilde{U}(1 - \delta_{\sigma,\sigma'}). \tag{15}$$

The quasiparticle or renormalized Green's function takes the form

$$\tilde{G}_\sigma(\omega) = \frac{1}{\omega - \tilde{\epsilon}_{\rm d} + \sigma h + {\rm i}\tilde{\Delta} - \tilde{\Sigma}_\sigma(\omega,h)}. \tag{16}$$

The reorganized perturbation theory is set up to calculate the renormalized self-energy $\tilde{\Sigma}_\sigma(\omega,h)$. The propagators in this expansion correspond to the non-interacting quasiparticles in the Lagrangian $\mathcal{L}_{\rm AM}(\bar{d}_\sigma, d_\sigma, \epsilon_{\rm d}, \Delta, U)$ with $\tilde{U} = 0$. The quasiparticle interaction $\tilde{U}$ is used as an expansion parameter but all the terms in the counter-Lagrangian $\mathcal{L}_{\rm CT}$ have to be included as well. To organize the expansion in powers of $\tilde{U}$, the terms λ_1, λ_2 and λ_3 have also to be expressed in powers of $\tilde{U}$:

$$\lambda_1 = \sum_{n=0}^{\infty}\lambda_1^{(n)}\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^n \qquad \lambda_2 = \sum_{n=0}^{\infty}\lambda_2^{(n)}\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^n \qquad \lambda_3 = \sum_{n=0}^{\infty}\lambda_3^{(n)}\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^n. \tag{17}$$

The coefficients $\lambda_1^{(n)}$, $\lambda_2^{(n)}$ and $\lambda_3^{(n)}$ are then determined by the requirement that the three normalization conditions (14) and (15) are satisfied by each order in the expansion. These normalization conditions are essentially those used within field theory in order to circumvent the problem of infinities arising from the lack of an ultraviolet cut-off (see for example [10]). The procedure, however, makes no mention of infinities; it simply allows the field theoretic perturbation expansion to be expressed in terms of the experimentally observed masses and interactions. In condensed matter systems divergences do not arise in this way, as there is always a natural cut-off, so there is no necessity to reorganize the perturbation expansion. However, for the Anderson model there are very strong renormalizations of the effective d level and the interactions at low energies in the Kondo regime, where the impurity d electrons are virtually localized, which make it desirable when working in this regime to take account of these very strong renormalizations from the start. This allows one to develop a perturbation theory with an effective d level and interactions appropriate to this energy scale. More generally it makes a direct link to Landau Fermi-liquid theory. There are no cut-off-dependent ultraviolet divergences to eliminate, so the question of the renormalizability of the model does not arise.

We can obtain significant results with this approach even at zero order, $\tilde{U} = 0$. If we calculate the quasiparticle occupation number $\tilde{n}_{\mathrm{d},\sigma}$ at $T = 0$ and $H = 0$ from (16) with $\tilde{U} = 0$, we find

$$\tilde{n}_{\mathrm{d},\sigma} = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\left(\frac{\tilde{\epsilon}_{\mathrm{d}}}{\tilde{\Delta}}\right). \tag{18}$$

As the factors of z in this expression cancel it is equivalent to the exact Friedel sum rule [12] and expresses the one-to-one correspondence between the quasiparticle number and electron number in Landau Fermi-liquid theory [14], $\tilde{n}_{\mathrm{d},\sigma} = n_{\mathrm{d},\sigma}$. Hence, the d-level occupation at $T = 0$ can be calculated from the zero-order renormalized Green's function.

The Friedel sum rule also holds in the presence of a magnetic field and the equivalent expression for the occupation of the d level in terms of the renormalized self-energy is given by

$$n_{\mathrm{d},\sigma} = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\left(\frac{\tilde{\epsilon}_{\mathrm{d}} - \sigma h + \tilde{\Sigma}_\sigma(0, h)}{\tilde{\Delta}}\right). \tag{19}$$

We have to use the perturbation theory to calculate the field dependence of the renormalized self-energy. However, we can show that it is sufficient to work only to first order in $\tilde{U}$ to obtain the exact result. There are two terms to first order, one from the tadpole or Hartree diagram and one from the corresponding counter-term diagram in λ_1. There is no wave-function renormalization to this order, so $\lambda_2^{(1)} = 0$, and also to this order $\tilde{\Gamma}_{\uparrow,\downarrow}(0, 0) = \tilde{U}$, so $\lambda_3^{(1)} = 0$. To satisfy the renormalization conditions the counter-term should cancel the contribution from the tadpole diagram for $T = h = 0$, so $\lambda_1 = \tilde{U} n^{(0)}_{\mathrm{d},-\sigma}(0, 0)$. Hence the combined contribution is

$$\tilde{\Sigma}^{(1)}_\sigma(\omega, h, T) = \tilde{U}(n^{(0)}_{\mathrm{d},-\sigma}(h, T) - n^{(0)}_{\mathrm{d},-\sigma}(0, 0)). \tag{20}$$

The spin susceptibility of the d electrons at $T = 0$ can be calculated from $g\mu_{\mathrm{B}}(n_{\mathrm{d},\uparrow} - n_{\mathrm{d},\downarrow})/2$, by substituting the self-energy from (20) into equation (19), and then differentiating with respect to H. The charge susceptibility can be calculated in a similar way and the two results are

$$\chi_{\mathrm{d}} = \frac{(g\mu_{\mathrm{B}})^2}{2}\tilde{\rho}_{\mathrm{d}}(0)(1 + \tilde{U}\tilde{\rho}_{\mathrm{d}}(0)) \qquad \chi_{\mathrm{d,c}} = 2\tilde{\rho}_{\mathrm{d}}(0)(1 - \tilde{U}\tilde{\rho}_{\mathrm{d}}(0)) \tag{21}$$

where $\tilde{\rho}_{\mathrm{d}}(0)$ is the quasiparticle density of states at the Fermi level and is given by

$$\tilde{\rho}_{\mathrm{d}}(0) = \frac{\tilde{\Delta}/\pi}{\tilde{\epsilon}_{\mathrm{d}}^2 + \tilde{\Delta}^2}. \tag{22}$$

It is not obvious that these results to first order in $\tilde{U}$ are exact. However, there are Ward identities [13] which can be derived from charge and spin conservation, and in terms of the renormalized self-energy and density of states take the form

$$\frac{\partial\tilde{\Sigma}_\sigma(\omega)}{\partial h}\bigg|_{\omega=0} = \frac{\partial\tilde{\Sigma}_\sigma(\omega)}{\partial \mu}\bigg|_{\omega=0} = -\tilde{\rho}_{\mathrm{d},\sigma}(0)\tilde{U}. \tag{23}$$

The spin and charge susceptibilities can be derived from these exact relations on using (19) to give

$$\chi_\mathrm{d} = \frac{(g\mu_\mathrm{B})^2}{2}\tilde{\rho}_\mathrm{d}(0)(1-\partial\tilde{\Sigma}/\partial h) = \frac{(g\mu_\mathrm{B})^2}{2}\tilde{\rho}_\mathrm{d}(0)(1+\tilde{U}\tilde{\rho}_\mathrm{d}(0)) \tag{24}$$

and

$$\chi_\mathrm{d,c} = 2\tilde{\rho}_\mathrm{d}(0)(1+\partial\tilde{\Sigma}/\partial\mu) = 2\tilde{\rho}_\mathrm{d}(0)(1-\tilde{U}\tilde{\rho}_\mathrm{d}(0)) \tag{25}$$

confirming that the first-order results for these quantities are indeed exact.

The impurity contribution to the low-temperature specific heat coefficient from the non-interacting quasiparticles ($\tilde{U}=0$) is given simply by

$$\gamma_\mathrm{d} = \frac{2\pi^2}{3}\tilde{\rho}_\mathrm{d}(0). \tag{26}$$

This result corresponds to the exact result calculated by Yamada [13]. It is a general feature of Fermi-liquid theory that the quasiparticle interactions do not give any corrections to the linear coefficient of specific heat as their contributions to the specific heat are of higher order in temperature.

In the local moment or Kondo regime the local charge susceptibility must go to zero, so from equation (21) we find $\tilde{U}\tilde{\rho}_\mathrm{d}(0) = 1$. If we define the Kondo temperature T_K by $\chi_\mathrm{d} = (g\mu_\mathrm{B})^2/4T_\mathrm{K}$ then $\tilde{\rho}_\mathrm{d}(0) = 1/4T_\mathrm{K}$ and all the results can be written in terms of T_K. They correspond to the exact results for the s–d or Kondo model [15, 16].

From the exact Bethe *ansatz* results [15, 16] for the spin and charge susceptibility for the symmetric Anderson model it is possible to deduce the renormalized parameters, $\tilde{\Delta}$ and $\tilde{U}$, in terms of the bare parameters Δ and U. These are shown in figure 1. Initially $\tilde{U}\sim U$ for small U, but when $U/\pi\Delta > 2$, the energy scales $\tilde{U}$ and $\pi\tilde{\Delta}$ merge in the strong-coupling regime and $\tilde{U} = \pi\tilde{\Delta} = 4T_\mathrm{K}$.

To calculate the low-temperature conductivity to order T^2 one needs to calculate the renormalized self-energy to order ω^2 and T^2. There is a T^2-contribution to the conductivity arising from the scattering of free quasiparticles by the impurity but there is an additional contribution due to the mutual scattering of the quasiparticles due to the inter-quasiparticle interactions. The lowest-order contribution of this type arises from the second-order diagram for $\tilde{\Sigma}$ shown in figure 2(b). The only counter-term diagram that has to be taken into account to order ω^2 or T^2 is due to the second term in $\lambda_2^{(2)}$, which is required to cancel the term linear in ω arising from the diagram in figure 2(b), and this gives $\lambda_2^{(2)} = 3-\pi^2/4$. We calculate this for the case of particle–hole symmetry which is such that $\tilde{\epsilon}_\mathrm{d} = -\tilde{U}/2$ and $n_\mathrm{d}(T) = 1$. The contribution to the imaginary part of the renormalized self-energy from figure 2(b) is

$$\mathrm{Im}\,\tilde{\Sigma}(\omega,T) = \pi\tilde{U}^2\int\tilde{\rho}_\mathrm{d}(\epsilon)\tilde{\rho}_\mathrm{d}(\epsilon')\tilde{\rho}_\mathrm{d}(\omega-\epsilon-\epsilon')D(\omega,\epsilon,\epsilon')\,\mathrm{d}\epsilon\,\mathrm{d}\epsilon' \tag{27}$$

where

$$D(\omega,\epsilon,\epsilon') = (1-f(\epsilon)-f(\epsilon'))f(\epsilon+\epsilon'-\omega)+f(\epsilon)f(\epsilon') \tag{28}$$

and $f(\epsilon)$ is the Fermi factor $1/(1+\mathrm{e}^{\beta\epsilon})$ with $\beta = 1/T$. To calculate the conductivity to order T^2 we need to evaluate this integral to order ω^2 for $T=0$. For $T=0$ equation (28) becomes

$$D(\omega,\epsilon,\epsilon') = (\theta(\epsilon)+\theta(\epsilon')-1)\theta(\omega-\epsilon-\epsilon')+(1-\theta(\epsilon))(1-\theta(\epsilon')) \tag{29}$$

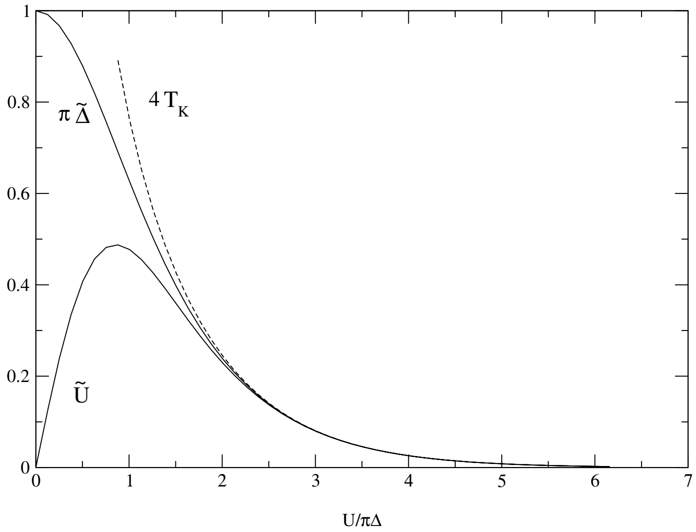

Figure 1. A plot of the renormalized parameters $\tilde{U}$ and $\pi\tilde{\Delta}$ for the symmetric Anderson model in terms of the bare parameters U and $\pi\Delta$. In the comparison of these parameters with $4T_{\rm K}$ for $U \gg \pi\Delta$ the value of $T_{\rm K}$ is given in equation (B.9).

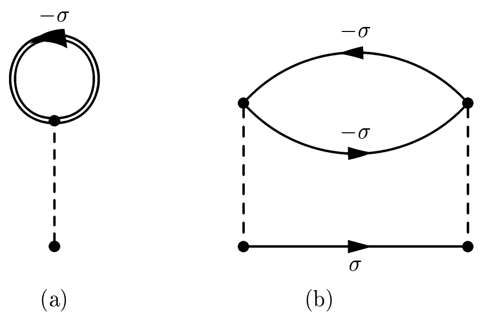

Figure 2. The skeleton tadpole diagram, (a), and second-order self-energy diagram, (b).

where $\theta(x)$ is the step function. To find the ω^2-coefficient we differentiate twice with respect to ω and use the relations

$$\frac{\partial\theta(x)}{\partial x} = \delta(x) \qquad \frac{\partial^2\theta(x)}{\partial x^2} = \delta'(x). \tag{30}$$

As $\tilde{\rho}_{\rm d}(0) = 1/\pi\tilde{\Delta}$ for the case of particle–hole symmetry, the result is

$$\mathrm{Im}\,\tilde{\Sigma}(\omega, 0) = -\frac{\pi}{2}\tilde{U}^2\tilde{\rho}_{\rm d}(0)^3\omega^2 = -\frac{\omega^2}{2\tilde{\Delta}}\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^2. \tag{31}$$

We need the corresponding results to order T^2 for $\omega = 0$. For $\omega = 0$ the temperature-dependent factor in the integrand of (28) is

$$D(0, \epsilon, \epsilon') = 2f(\epsilon)f(\epsilon')(1 - f(\epsilon + \epsilon')). \tag{32}$$

We can change the variables of integration to x and x', where $x = \epsilon T$ and $x' = \epsilon' T$, and the integral of equation (27) to order T^2 becomes

$$\mathrm{Im}\,\tilde{\Sigma}(0, T) = -\frac{T^2}{\tilde{\Delta}}\left(\frac{U}{\pi\tilde{\Delta}}\right)^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} 2F(x)F(x')(1 - F(x + x'))\,\mathrm{d}x\,\mathrm{d}x' \tag{33}$$

where $F(x) = 1/(1 + e^x)$. The integration over x' can be carried out to give

$$\mathrm{Im}\,\tilde{\Sigma}(0, T) = \frac{T^2}{\tilde{\Delta}}\left(\frac{U}{\pi\tilde{\Delta}}\right)^2 \int_{-\infty}^{\infty} \frac{x}{\sinh x}\,\mathrm{d}x = \frac{\pi^2 T^2}{2\tilde{\Delta}}\left(\frac{U}{\pi\tilde{\Delta}}\right)^2. \tag{34}$$

To evaluate the conductivity we need to evaluate the transport relaxation lifetime $\tau(\omega, T)$ which is proportional to the inverse of the impurity density of states $\rho_{\mathrm{d}}(\omega, T)$ which in turn is proportional to the imaginary part of the renormalized Green's function, so

$$\tau(\omega, T) \propto \pi\tilde{\rho}_{\mathrm{d}}(\omega, T)^{-1} = \tilde{\Delta} - \mathrm{Im}\,\tilde{\Sigma}(\omega, T) + \frac{(\omega - \mathrm{Re}\,\tilde{\Sigma}(\omega, T))^2}{(\tilde{\Delta} - \mathrm{Im}\,\tilde{\Sigma}(\omega, T))}. \tag{35}$$

When these results are used to evaluate the contribution to the impurity conductivity $\sigma_{\mathrm{imp}}(T)$ to order T^2 we find

$$\sigma_{\mathrm{imp}}(T) = \sigma_0\left\{1 + \frac{\pi^2}{3}\left(\frac{T}{\tilde{\Delta}}\right)^2(1 + 2(R-1)^2) + \mathrm{O}(T^4)\right\} \tag{36}$$

where R is the Wilson ratio given by $R = 1 + \tilde{U}/\pi\tilde{\Delta}$. This is an exact result to order T^2 which was first derived by Nozières [17] for the Kondo regime, which corresponds to $\tilde{U} = \pi\tilde{\Delta} = 4T_{\mathrm{K}}$ and $R = 2$. The more general result was derived by Yamada [13]. More recently Lesage and Saleur [18] have also calculated the coefficients of the T^4- and T^6-terms in this expansion in the Kondo regime, using boundary conformal field theory.

Nothing has been omitted in the renormalized perturbation expansion, and it gives the asymptotically exact results in the low-temperature regime, when taken to second order in $\tilde{U}$, so it would be interesting to extend the results by including higher-order terms. One possibility would be to include all the terms to fourth order in $\tilde{U}$, and calculate the coefficient of the next correction term in the conductivity, the T^4-term, to compare the result with that of Lesage and Saleur. However, this would be require an expansion of the self-energy in terms of both the frequency and temperature for all the fourth-order terms, which, though straightforward to carry out, would be a rather long and tedious exercise. An alternative way of examining the contributions from the next-order terms would be to calculate the H^3-term in the field dependence of the impurity magnetization in a weak magnetic field. The linear term in H was given exactly by the first-order renormalized expansion. The coefficient of the H^3-term is known exactly for the Kondo model at $T = 0$, and also for the symmetric Anderson model, from Bethe *ansatz* calculations [15, 16]. The renormalized perturbation calculation of this coefficient to order $\tilde{U}^3$ is described in the next section.

3. Higher-order terms

We will perform the renormalized perturbation calculations here in a way slightly different but equivalent to the one used in the previous section. It will have the advantage of not involving the explicit use of counter-terms. We will also obtain an expression for the renormalized parameters in terms of the bare ones, at least for weak coupling. We first of all use the standard perturbation theory in U, and then calculate the renormalized parameters explicitly to the appropriate order. We can invert this relation and then write the standard perturbation result in terms of the renormalized parameters, i.e. we renormalize the standard perturbation terms order by order using the renormalization conditions (10) and (11). The result will correspond to the renormalized expansion in $\tilde{U}$, as described in the previous section, when taken to the same order.

3.1. Third-order perturbation theory

We use the zero-temperature formalism where the impurity Green's function can be written in the form

$$G_\sigma(\omega, h) = \frac{1}{\omega - \epsilon_{\rm d} + \sigma h + {\rm i}\Delta\,{\rm sgn}(\omega) + \Sigma_\sigma(\omega, h)} \tag{37}$$

where $h = g\mu_{\rm B}H/2$. An expression for the impurity magnetization in terms of the magnetic field-dependent self-energy at $T = 0$ can be derived from the Friedel sum rule, where the impurity level occupation number $n_{{\rm d},\sigma}$ in the spin channel σ is given by

$$n_{{\rm d},\sigma} = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\left(\frac{\epsilon_{\rm d} - \sigma h + \Sigma_\sigma(0, h)}{\Delta}\right) \tag{38}$$

which is equivalent to equation (19). We can deduce from this an expression for the induced impurity magnetization, and expand it to order h^3. However, it will be useful to separate out the skeleton tadpole diagram shown in figure 2(a), which has the full Green's function, indicated by a double propagator, in the bubble, as this is equal to $Un_{{\rm d},-\sigma}$, where $n_{{\rm d},-\sigma}$ is the exact expectation value of the occupation number. We write the self-energy $\Sigma_\sigma(\omega, h)$ in the form

$$\Sigma_\sigma(\omega, h) = Un_{{\rm d},-\sigma} + \bar{\Sigma}_\sigma(\omega, h) \tag{39}$$

and substitute it into equation (38). We write the impurity magnetization $M(h) = g\mu_{\rm B}(n_{{\rm d},\uparrow} - n_{{\rm d},\downarrow})/2$ in a weak field as a power series:

$$M(h) = \frac{g\mu_{\rm B}}{\pi}\sum_n M_{2n+1}\left(\frac{h}{\Delta}\right)^{2n+1}. \tag{40}$$

For the particle–hole-symmetric model ($\epsilon_{\rm d} = -U/2$) these coefficients in terms of the self-energy $\bar{\Sigma}_\uparrow(0, h)$ are

$$M_1 = \frac{1}{(1 - U/\pi\Delta)}\left(1 - \left.\frac{\partial\bar{\Sigma}_\uparrow(0, h)}{\partial h}\right|_{h=0}\right) \tag{41}$$

$$M_3 = -\frac{1}{3(1 - U/\pi\Delta)}\left(M_1^3 + \frac{\Delta^2}{2}\left.\frac{\partial^3\bar{\Sigma}_\uparrow(0, h)}{\partial^3 h}\right|_{h=0}\right). \tag{42}$$

We have the results for the first derivative of the self-energy with respect to h to order U^3 from the calculations of Yamada [13]:

$$M_1 = 1 + \frac{U}{\pi\Delta} + \left(3 - \frac{\pi^2}{4}\right)\left(\frac{U}{\pi\Delta}\right)^2 + \left(15 - \frac{3\pi^2}{2}\right)\left(\frac{U}{\pi\Delta}\right)^3. \tag{43}$$

The only unknown term in the expression for the third-order magnetization to order U^3 is the third-order derivative of the self-energy at zero frequency with respect to the magnetic field h.

To second order in U there is only one diagram which contributes to $\bar{\Sigma}_\sigma(\omega, h)$, that shown in figure 2(b), which gives a contribution

$$\bar{\Sigma}_\uparrow^{(2b)}(\omega, h) = U^2\int G_\uparrow^{(0)}(\omega - \omega', h)\Pi^{p\downarrow,h\downarrow}(\omega', h)\,\frac{{\rm d}\omega'}{2\pi{\rm i}}. \tag{44}$$

The particle–hole propagator $\Pi^{p\sigma,h\sigma'}$ and the corresponding particle–particle propagator $\Pi^{p\sigma,h\sigma'}$ are both evaluated in appendix A.

$$\bar{\Sigma}_\uparrow^{(2b)}(0, h) = -h\left(2 - \frac{\pi^2}{4}\right)\left(\frac{U}{\pi\Delta}\right)^2 + \frac{Ch^3}{3\Delta^2}\left(\frac{U}{\pi\Delta}\right)^2 \tag{45}$$

where the coefficient C has been evaluated numerically, and we find a value $C \approx -1.735$.

The third-order diagrams fall into two types. There are three diagrams shown in figure 3 corresponding to dressing each of the propagators in the second-order self-energy diagram with a simple tadpole or zero-order Hartree term. For the symmetric model the contributions from the first two diagrams, figures 3(a) and 3(b), cancel to first order in h but contribute to higher order. The contribution from the diagram 3(a) in which the particle line is dressed with a tadpole is

$$\tilde{\Sigma}^{(3a)}_{\uparrow}(\omega, h) = \frac{U^3}{\pi}\tan^{-1}\left(\frac{h}{\Delta}\right)\int (G^{(0)}_{\downarrow}(\omega-\omega', h))^2\Pi^{p\uparrow,h\downarrow}(\omega', h)\,\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \quad (46)$$

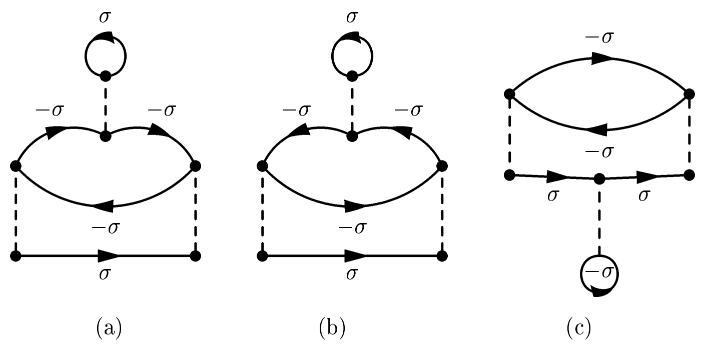

Figure 3. Third-order diagrams with a tadpole insertion.

The contribution from the corresponding diagram 3(b) in which the spin-down hole line is dressed is

$$\tilde{\Sigma}^{(3b)}_{\uparrow}(\omega, h) = \frac{U^3}{\pi}\tan^{-1}\left(\frac{h}{\Delta}\right)\int (G^{(0)}_{\downarrow}(-\omega+\omega', h))^2\Pi^{p\uparrow,p\downarrow}(\omega', h)\,\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \quad (47)$$

As $\Pi^{p\uparrow,p\downarrow}(\omega', h) = -\Pi^{p\downarrow,h\downarrow}(\omega', h)$ and $G^{(0)}_{\downarrow}(-\omega+\omega', h) = -G^{(0)}_{\uparrow}(\omega-\omega', -h)$, we can rewrite this contribution as

$$\tilde{\Sigma}^{(3b)}_{\uparrow}(\omega, h) = -\frac{U^3}{\pi}\tan^{-1}\left(\frac{h}{\Delta}\right)\int (G^{(0)}_{\downarrow}(\omega-\omega', -h))^2\Pi^{p\downarrow,h\downarrow}(\omega', h)\,\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \quad (48)$$

We are left with the contribution from the diagram in figure 3(c) in which the spin-$\uparrow$ propagator of a particle–hole bubble is dressed with a Hartree bubble:

$$\tilde{\Sigma}^{(3c)}_{\uparrow}(\omega, h) = -\frac{U^3}{\pi}\tan^{-1}\left(\frac{h}{\Delta}\right)\int (G^{(0)}_{\uparrow}(\omega-\omega', h))^2\Pi^{p\downarrow,h\downarrow}(\omega', h)\,\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \quad (49)$$

The total result from the three diagrams to order h^3 is

$$\tilde{\Sigma}^{(3)}_{\uparrow}(0, h) = -h\left(2-\frac{\pi^2}{4}\right)\left(\frac{U}{\pi\Delta}\right)^3 + \frac{Eh^3}{3\Delta^2}\left(\frac{U}{\pi\Delta}\right)^3 \quad (50)$$

where the coefficient E is calculated numerically as -5.670.

Finally there are the two diagrams illustrated in figures 4(a) and 4(b), which can be regarded as being derived from the second-order diagram, figure 2(b), with an intermediate scattering in the subdiagram corresponding to one of the dynamic susceptibilities. The contribution from the diagram in figure 4(a) is

$$\tilde{\Sigma}^{(4a)}_{\uparrow}(\omega, h) = -U^3\int G^{(0)}_{\downarrow}(\omega-\omega', h)(\Pi^{p\uparrow,h\downarrow}(\omega', h))^2\,\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}} \quad (51)$$

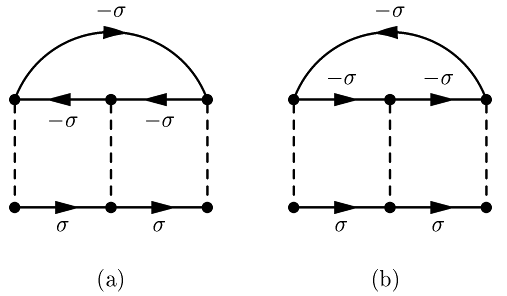

Figure 4. Third-order diagrams with repeated particle–hole scattering, (a), and particle–particle scattering, (b).

with intermediate particle–hole scattering. For the diagram in figure 4(b) with intermediate particle–particle scattering the contribution is

$$\bar{\Sigma}_{\uparrow}^{(4b)}(\omega, h) = -U^3 \int G_{\downarrow}^{(0)}(\omega' - \omega, h)(\Pi^{p\uparrow,p\downarrow}(\omega', h))^2 \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \tag{52}$$

The total result is

$$\bar{\Sigma}_{\uparrow}^{(4a)}(0, h) + \bar{\Sigma}_{\uparrow}^{(4b)}(0, h) = -h(10 - \pi^2)\left(\frac{U}{\pi\Delta}\right)^3 + \frac{Dh^3}{3\Delta^2}\left(\frac{U}{\pi\Delta}\right)^3. \tag{53}$$

The coefficient D was estimated numerically as $D = 1.541$.

Collecting the results to third order in U together,

$$M_3 = -\left\{1 + 4\frac{U}{\pi\Delta} + A\left(\frac{U}{\pi\Delta}\right)^2 + B\left(\frac{U}{\pi\Delta}\right)^3\right\} \tag{54}$$

$$A = 16 - \frac{3\pi^2}{4} + C \qquad B = 80 - \frac{27\pi^2}{4} + C + D + E. \tag{55}$$

The coefficients A and B can also be deduced from the Bethe *ansatz* results for the magnetization of the symmetric Anderson model by generalizing the approach of Horvatić and Zlatić [19], who derived a recurrence relation for a series expansion in powers of U for the coefficient M_1, to obtain a similar expansion for M_3. The details are given in appendix B. We find $A = 65/3 - 3\pi^2/2$ which gives $C = 17/3 - 3\pi^2/4 = -1.7355$, in complete agreement with the numerical estimate, and $B = 15(280/27 - \pi^2) = 7.512$, which agrees well the numerical estimate 7.515.

3.2. Renormalization

Having calculated all the self-energy terms to order U^3 using the standard perturbation theory we want to deduce the corresponding results in the renormalized expansion to order $\tilde{U}^3$.

We need to calculate the renormalized parameters, $\tilde{\Delta}$ and $\tilde{U}$, using the definitions given in equations (10) and (11), in terms of the bare parameters to order U^3. For this we will need the wavefunction renormalization factor z and the irreducible four-point vertex function $\Gamma_{\uparrow,\downarrow}(0, 0, 0, 0)$. The only contribution to z to order U^3 comes from the second-order diagram and the result is

$$z = 1 - \left(3 - \frac{\pi^2}{4}\right)\left(\frac{U}{\pi\Delta}\right)^2 + \mathrm{O}\left[\left(\frac{U}{\pi\Delta}\right)^4\right] \tag{56}$$

which can also be deduced from the results in Yamada's paper [13]. The contributions from the diagrams for the irreducible vertex function $\Gamma_{\uparrow,\downarrow}(0,0,0,0)$ to second order in U cancel in the absence of a magnetic field. Diagrams which contribute at third order in U are shown in figure 5. There are three possible diagrams of the type shown in figure 5(a) each one giving a contribution $U(U/\pi\Delta)^2$. There are six other diagrams in all of the type shown in figures 5(b) and 5(c), and each of these gives a contribution $(2-\pi^2/4)U(U/\pi\Delta)^2$. The total to third order in U is

$$\Gamma_{\uparrow,\downarrow}(0,0,0,0) = U\left\{1+\left(15-\frac{3\pi^2}{2}\right)\left(\frac{U}{\pi\Delta}\right)^2+\cdots\right\}. \qquad (57)$$

From these two results we can deduce the renormalized parameters to order U^3:

$$\tilde{\Delta} = \Delta\left\{1-\left(3-\frac{\pi^2}{4}\right)\left(\frac{U}{\pi\Delta}\right)^2+\cdots\right\} \qquad \tilde{U} = U\left\{1-(\pi^2-9)\left(\frac{U}{\pi\Delta}\right)^2+\cdots\right\}. \qquad (58)$$

These results correspond to the weak-coupling region $U \ll \pi\Delta$ in the plot of the renormalized parameters shown in figure 1.

We can invert these expression to deduce the bare parameters Δ and U in terms of the renormalized ones, $\tilde{\Delta}$ and $\tilde{U}$:

$$\Delta = \tilde{\Delta}\left\{1+\left(3-\frac{\pi^2}{4}\right)\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^2+\cdots\right\} \qquad U = \tilde{U}\left\{1+(\pi^2-9)\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^2+\cdots\right\}. \qquad (59)$$

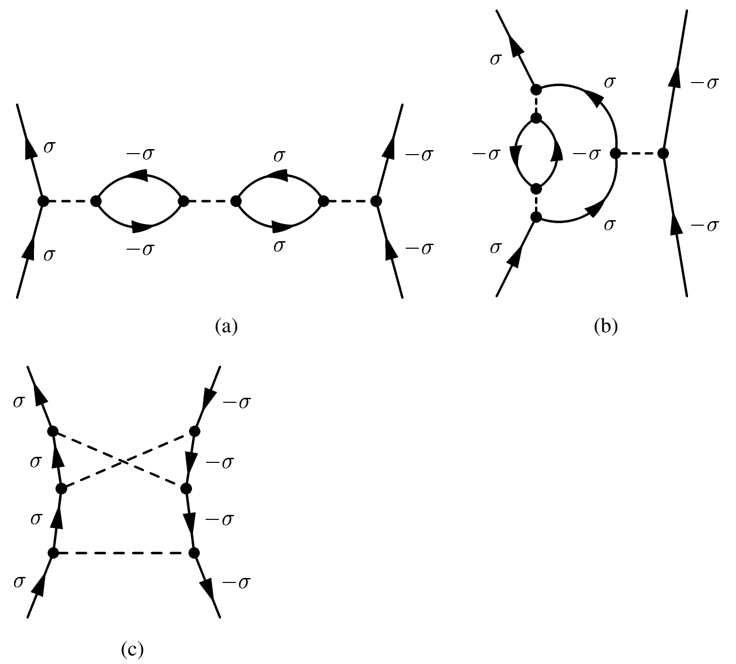

Figure 5. Third-order contributions to the irreducible four-vertex $\Gamma_{\uparrow,\downarrow}(0,0,0,0)$.

We now use these relations to express the third-order result in U for the magnetization in terms of the renormalized parameters. It will be convenient to write (40) in a modified form:

$$M(h) = \frac{g\mu_B}{\pi}\sum_n \tilde{M}_{2n+1}\left(\frac{h}{\tilde{\Delta}}\right)^{2n+1}. \qquad (60)$$

The coefficient $\tilde{M}_3$ to third order in $\tilde{U}$ is given by

$$\tilde{M}_3 = \left\{1 + 4\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right) + A'\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^2 + B'\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^3\right\} \tag{61}$$

where

$$A' = 7 + C \qquad B' = \frac{5\pi^2}{4} - 4 + C + D + E. \tag{62}$$

We know from the Ward identity (23) that the result to order h is exact to all orders in $\tilde{U}$. We know that the term of order h^3 is asymptotically exact in the weak-coupling regime, $U/\pi\Delta \to 0$, so it is of interest to check it in the strong-coupling limit against exact Bethe *ansatz* results for the Kondo model. We use the results in the previous section to express all of the renormalized parameters in terms of the Kondo temperature T_K: $\tilde{U}/\pi\tilde{\Delta} \to 1$ and $\pi\tilde{\Delta} \to 4T_K$ as $U \to \infty$. We then find

$$\frac{M(h)}{g\mu_B} = \frac{h}{2T_K} - D'\frac{h^3\pi^2}{192T_K^3} \tag{63}$$

where $D' = 5 + A' + B' = 8 + 5\pi^2/4 + 2C + D + E$. With the values of the coefficients as deduced from the third-order renormalized perturbation theory, we get $D' = 12.73$. If the exact Bethe *ansatz* result is written in the same form, using the same definition of T_K, the coefficient D' has the value $D' = 24\sqrt{3}/\pi = 13.232$. The error from our third-order results is less than 4%. Hence the perturbation theory taken to third order, which is asymptotically exact in the weak-coupling regime, is very close to the exact result for strong coupling.

As $\tilde{U}/\pi\tilde{\Delta} \to 1$ in the strong-coupling limit, the factor $(\tilde{U}/\pi\tilde{\Delta})^n$ multiplying the contributions from the nth-order terms do not decrease with n, as they do in the weak-coupling limit $\tilde{U}/\pi\tilde{\Delta} \ll 1$. In appendix B we show that in the Kondo limit no finite set of renormalized diagrams can give the h^3-coefficient in the magnetization exactly. However, we have shown that the error is small in the limit where the perturbation series is taken to third order, and is even smaller for intermediate and weak coupling. This is clearly seen from the results in figure 6 where we plot the coefficient $\tilde{M}_3$ against $\tilde{U}/\pi\tilde{\Delta}$ over the range from weak ($\tilde{U}/\pi\tilde{\Delta} \ll 1$) to strong coupling ($\tilde{U}/\pi\tilde{\Delta} = 1$) as calculated from the third-order renormalized

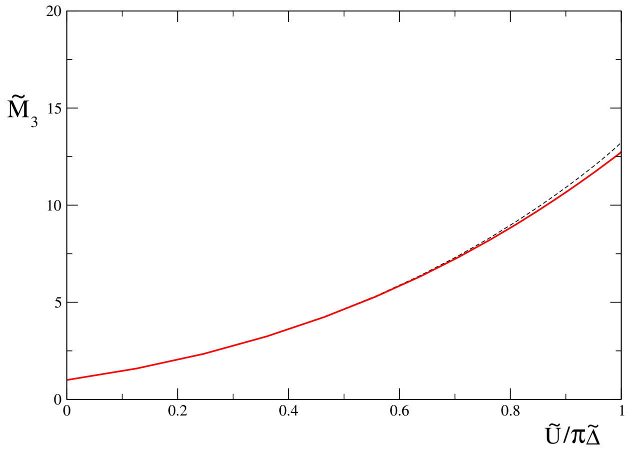

Figure 6. The coefficient $\tilde{M}_3$ from the third-order renormalized calculation compared with the exact Bethe *ansatz* result (dotted line) plotted as a function of $\tilde{U}/\pi\tilde{\Delta}$.

perturbation theory and compare it with the exact Bethe *ansatz* results, expressed in terms of the renormalized parameters $\tilde{U}$ and $\tilde{\Delta}$. Over the range from $U = \tilde{U} = 0$ to $U = 5\pi\Delta$ ($0 < \tilde{U}/\pi\tilde{\Delta} \leqslant 0.9998$), $\tilde{\Delta}/\Delta$ varies by two orders of magnitude, from 1 to $\sim 8 \times 10^{-3}$.

It would be interesting if there were some way of extracting the small h^3-correction from the higher-order diagrams. We have taken account of the contribution from the leading-order irrelevant term ($\tilde{U}$) about the low-energy fixed point to third order, so the remaining contributions must be related to the next-order irrelevant terms in the effective Hamiltonian at the Wilson strong-coupling fixed point. These terms must be a combination of local operators but it is not clear how to relate these explicitly to the higher-order diagrams in the renormalized perturbation theory.

4. Dynamic response functions in a weak magnetic field

If we calculate the ω-dependence of the self-energy as well as the h-dependence we can deduce the form of the quasiparticle density of states in a weak magnetic field. If we calculate this as a general function of ω and h, rather than expanding in powers of ω and h, it will be more convenient to revert to the renormalized expansion as used in section 2 with the explicit use of counter-terms. This just requires a rearrangement of the terms calculated in the previous section. Each diagram will now be interpreted as a diagram for the renormalized self-energy $\tilde{\Sigma}_\sigma(\omega, h)$, with $U \to \tilde{U}$ and $\Delta \to \tilde{\Delta}$, and $\tilde{\epsilon}_d = -\tilde{U}/2$, but we will have to include the counter-terms to order $\tilde{U}^3$ to satisfy the renormalization conditions. For the particle–hole-symmetric model, the only non-zero counter-terms to third order are: $\lambda_1 = 0$, $\lambda_2^{(2)} = 3 - \pi^2/4$ and $\lambda_3^{(3)} = -\pi\tilde{\Delta}(15 - 3\pi^2/2)$. The only new term to order $\tilde{U}^3$ is the last term which cancels off the renormalization of the four-vertex $\tilde{\Gamma}_{\uparrow,\downarrow}(0, 0, 0, 0)$ shown in figure 5, which is not needed, as the vertex $\tilde{U}$ is taken to be the fully renormalized one. An alternative way to calculate the counter-terms is directly from their definitions in terms of the self-energy and vertex functions, and to re-express these in terms of the renormalized parameters.

The counter-term diagrams are shown in figure 7. The first diagram, figure 7(a), involves the λ_2-vertex, and ensures that the linear term in ω is cancelled off. The next diagram, figure 7(b), is an additional tadpole contribution arising from the counter-term interaction λ_3. There is also a third-order counter-term diagram, figure 7(c), arising from a combination of the tadpole diagram to order $\tilde{U}$ with a counter-term vertex λ^2 on the bubble. This diagram gives a contribution

$$\Sigma_\uparrow^{\mathrm{ct}}(\omega, h) = \left(3 - \frac{\pi^2}{4}\right)\tilde{U}\left(\frac{\tilde{U}}{\pi\tilde{\Delta}}\right)^2 \int (\omega' + h)(G_\downarrow^{(0)}(\omega', h))^2 \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \tag{64}$$

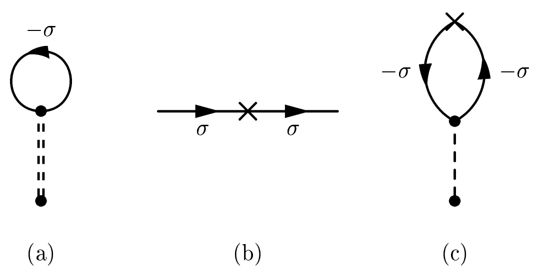

Figure 7. Counter-term diagrams which contribute to the self-energy to third order in $\tilde{U}$. The double-dashed line represents the vertex λ_3, the cross represents the vertex λ_2 and the single-dashed line represents $\tilde{U}$.

The evaluation of the integral is straightforward and gives

$$\Sigma^{\rm ct}_{\uparrow}(\omega,h)=\tilde\Delta\left(3-\frac{\pi^2}{4}\right)\left(\frac{\tilde U}{\pi\tilde\Delta}\right)^3\left[\tan^{-1}\left(\frac{h}{\tilde\Delta}\right)-\frac{\tilde\Delta h}{h^2+\tilde\Delta^2}\right]. \tag{65}$$

If the self-energy to third order from the standard diagrams calculated in the previous section in terms of the renormalized parameters ($U\to\tilde U$, $\Delta\to\tilde\Delta$) is written as $\Sigma^{(3)}_{\uparrow}(\omega,h)$, then the renormalized self-energy to order $\tilde U^3$ is given by

$$\tilde\Sigma^{(3)}_{\uparrow}(\omega,h)=\Sigma^{(3)}_{\uparrow}(\omega,h)+\tilde\Delta\left(15-\frac{3\pi^2}{2}\right)\tan^{-1}\left(\frac{h}{\tilde\Delta}\right)\left(\frac{\tilde U}{\pi\tilde\Delta}\right)^3+(\omega+h)\left(3-\frac{\pi^2}{4}\right)\left(\frac{\tilde U}{\pi\tilde\Delta}\right)^2$$
$$-\tilde\Delta\left(3-\frac{\pi^2}{4}\right)\left[\tan^{-1}\left(\frac{h}{\tilde\Delta}\right)-\frac{\tilde\Delta h}{h^2+\tilde\Delta^2}\right]\left(\frac{\tilde U}{\pi\tilde\Delta}\right)^3. \tag{66}$$

One can check that, in the limit $\omega=0$ and expanded to order h^3, this renormalized self-energy, when substituted into equation (19), gives the same results for the magnetization as were obtained in the previous section.

In figure 8 we plot the quasiparticle spectral densities in weak and strong coupling as a function of $\omega/\tilde\Delta$ for $h=0.15\tilde\Delta$. The peaks in the spectral density shift from $\omega_{\rm max}=\pm h$ for weak coupling to $\omega_{\rm max}=\pm 4h/3$ for strong coupling. These are asymptotically exact results as $h\to 0$, as has been shown by Logan and Dickens [20]. The general result for the position of the maximum in weak field from their calculation can be written in the form

$$\omega_{\rm max}=\frac{\pm 2h(1+\tilde U/[\pi\tilde\Delta])}{2+(\tilde U/[\pi\tilde\Delta])^2}. \tag{67}$$

The term in $\tilde U^2$ in the denominator arises from the contribution from the imaginary part of the self-energy at low frequency. The peak in the spectral density in the strong-coupling $\tilde U/\pi\tilde\Delta=1$ or localized limit, is the Kondo resonance, which has a width $\tilde\Delta=4T_{\rm K}/\pi$.

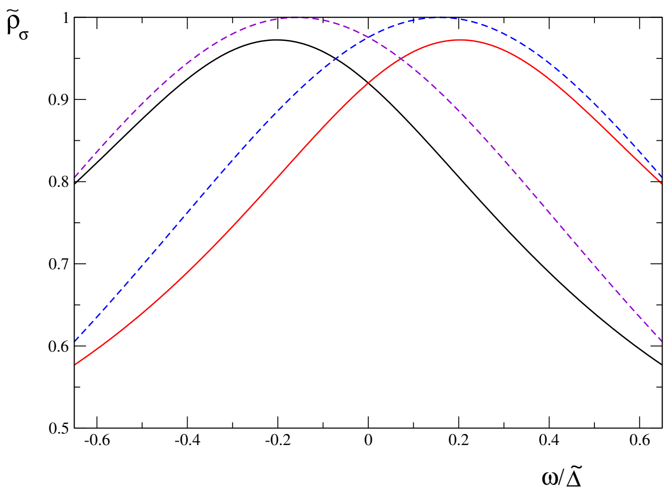

Figure 8. The density of states for ↑ and ↓ quasiparticles in a magnetic field $h/\tilde\Delta=0.15$ for weak coupling $\tilde U/\pi\tilde\Delta=0.1$ (dotted curves) and strong coupling $\tilde U/\pi\tilde\Delta=1.0$ plotted as a function of $\omega/\tilde\Delta$.

There have been a number of recent calculations of the Kondo resonance in a magnetic field for the Anderson model. The surge of interest in this topic has been due to the recent observations of the Kondo effect in quantum dots [21, 22]. These mesoscopic systems can be described by an impurity Anderson model coupled by leads to two electron reservoirs, and tunnelling through these dots at very low temperatures is possible due to the presence of the Kondo resonance. As the parameters in the Anderson model description of a quantum dot depend upon gate voltages, they can be modified in a much more controlled way than for real magnetic impurities, which should present a greater range of possibilities for comparing theory with experiment. There have been numerical renormalization group calculations of the Kondo resonance in a magnetic field [23, 24], approximate treatments based on the Bethe *ansatz* equations [25, 26] and also results from the local moment approach [27]. The advantage of the renormalized perturbation approach is that the results are asymptotically exact in the limits of small ω and H, and form a useful check on the other methods.

5. Conclusions

We have shown that the renormalized perturbation theory (RPT) approach provides a way of going beyond the normal limitations of standard perturbation theory. The potential of this approach has been illustrated in the particular case of the Anderson impurity model, where we have shown that low-order RPT calculations provide a comprehensive description of the low-energy, low-temperature range, in the Kondo as well as the weak-coupling regime. Except in the weak-coupling regime, we do not have explicit expressions for the renormalized parameters in terms of the bare ones (other than deducing them from the Bethe *ansatz* results; see figure 1), but this is also true of other approaches to magnetic impurity problems such as the conformal field theory [18]. There may be ways of estimating the renormalized parameters using variational methods, numerically, or by the summing a subset of diagrams, as in the local moment approach which gives a good approximate interpolation from weak to strong coupling. The RPT approach does give a clear physical picture of the Fermi-liquid regime, and the low-order results are asymptotically exact in this limit. This is also the case for other magnetic impurity models that have been studied, which include degeneracy and extra interactions, such as a Hund's rule coupling, and explicit expressions have been derived for the renormalized interactions in terms of the Kondo temperature, in the strong-coupling limit [7, 28]. It provides a complementary approach to the Wilson style of calculations which involve the explicit elimination of higher-order excitations [29, 30].

Two obvious questions arise: Can it be applied to lattice models? Is it applicable to systems with a non-Fermi-liquid fixed point? The method has also already been extended to translationally invariant systems [31], and related to Fermi-liquid theory. It is an alternative to the Wilson style of renormalization group approach, which has been applied to translationally invariant systems at one-loop level by Shankar [32]. There is potential for applications here, using the technique described in section 3: applying the RPT approach to the strong-coupling regime for such models as the Hubbard and periodic Anderson models. The complications that arise for translationally invariant systems and lattice models are mainly due to the dependence of the self-energy and renormalized vertices on the wave vector $\boldsymbol{k}$. There should be some simplification that one could exploit for infinite-dimensional models where the self-energy is $\boldsymbol{k}$-independent, and the $\boldsymbol{k}$-dependence is suppressed at some types of vertex.

The assumption of a finite wavefunction renormalization factor z in the derivation of the renormalized expansion restricts our treatment to Fermi liquids. Deviations from Fermi-liquid behaviour can have various causes and each case has to be considered on its own merits. It has proved possible to generalize the approach to a spinless Luttinger liquid [31], and to the O(3) symmetric Anderson model, which has a marginal Fermi-liquid fixed point [33].

Acknowledgments

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Appendix A

There are two types of subdiagrams which correspond to zero-order spin susceptibilities, with propagators defined by

$$\Pi^{p\sigma,h\sigma'}(\omega,h)=\int_{-\infty}^{\infty}G_{\sigma}^{(0)}(\omega+\omega',h)G_{\sigma'}^{(0)}(\omega',h)\,\frac{d\omega'}{2\pi i} \tag{A.1}$$

and

$$\Pi^{p\sigma,p\sigma'}(\omega,h)=\int_{-\infty}^{\infty}G_{\sigma}^{(0)}(\omega-\omega',h)G_{\sigma'}^{(0)}(\omega',h)\,\frac{d\omega'}{2\pi i}. \tag{A.2}$$

These integrals can be evaluated analytically and the results are

$$\Pi^{p\uparrow,h\uparrow}(\omega,h)=\begin{cases}\dfrac{-\Delta}{\pi(h^2+\Delta^2)} & \text{for } \omega=0\\ \dfrac{\Delta}{\pi\omega(\omega+2i\Delta)}\left\{\ln\left(\dfrac{\omega+i\Delta-h}{i\Delta-h}\right)+\ln\left(\dfrac{\omega+i\Delta+h}{i\Delta+h}\right)\right\} & \text{for } \omega\neq 0.\end{cases} \tag{A.3}$$

and

$$\Pi^{p\uparrow,h\downarrow}(\omega,h)=\begin{cases}\dfrac{1}{2\pi\Delta}\ln\left(\dfrac{i\Delta-h}{i\Delta+h}\right)-\dfrac{i}{\pi(i\Delta-h)} & \text{for } \omega=-2h\\ i\dfrac{\Delta}{\pi}\left\{\dfrac{1}{\omega+2h+2i\Delta}\ln\left(\dfrac{\omega+i\Delta+h}{i\Delta+h}\right)\right. & \\ \qquad\left.-\dfrac{1}{\omega+2h}\ln\left(\dfrac{\omega+i\Delta+h}{i\Delta-h}\right)\right\} & \text{for } \omega\neq -2h.\end{cases} \tag{A.4}$$

For particle–hole symmetry, we have $\Pi^{p\uparrow,p\downarrow}(\omega,h)=-\Pi^{p\downarrow,h\downarrow}(\omega,h)$ and $\Pi^{p\downarrow,h\downarrow}(\omega,h)=\Pi^{p\uparrow,h\uparrow}(\omega,h)=\Pi^{p\downarrow,h\downarrow}(\omega,-h)$.

Appendix B

In this appendix we take the expression for the magnetization from the exact Bethe *ansatz* results of Tsvelik and Wiegmann [16] for the symmetric Anderson model, and deduce a power series in U for the coefficient of the term in H^3, along the same lines at that originally used by Horvatić and Zlatić [19] for the order-H term. The result for the magnetization to order h^3 can be written in the form

$$\frac{\pi\Delta M(h)}{g\mu_B h}=\left(1-\frac{h^2}{2u\Delta^2}\right)e^{\pi^2u/8}J_1(u)+\frac{h^2}{2u\Delta^2}e^{3\pi^2u/8}J_3(u) \tag{B.1}$$

where $u=U/\pi\Delta$ where

$$J_m(u)=\sqrt{\frac{2m}{\pi u}}\int_0^{\infty}e^{-mx^2/2u}\frac{\cos(m\pi x/2)}{1-x^2}\,dx. \tag{B.2}$$

Horvatić and Zlatić have developed a power series in u for $J_1(u)$:

$$J_1(u) = \sum_{n=0} C_n u^n \qquad \text{where } C_n = (2n-1)C_{n-1} - \frac{\pi^2}{4}C_{n-2} \tag{B.3}$$

with $C_0 = C_1 = 1$ and $C_2 = 3 - \pi^2/4$. The other coefficients to order u^5 are

$$C_3 = 15 - \frac{3\pi^2}{4} \qquad C_4 = 105 - \frac{45\pi^2}{4} + \frac{\pi^4}{16} \qquad C_5 = 15\left(63 - 7\pi^2 + \frac{\pi^4}{16}\right). \tag{B.4}$$

We can develop an expansion for $J_3(u)$ in a similar way:

$$J_3(u) = \sum_{n=0} \bar{C}_n u^n \qquad \text{where } \bar{C}_n = \frac{(2n-1)}{3}\bar{C}_{n-1} - \frac{\pi^2}{4}\bar{C}_{n-2} \tag{B.5}$$

with $\bar{C}_0 = 1$, $\bar{C}_1 = 1/3$, $\bar{C}_2 = 1/3 - \pi^2/4$ and

$$\bar{C}_3 = \frac{5}{9} - \frac{\pi^2}{2} \qquad \bar{C}_4 = \frac{35}{27} - \frac{5\pi^2}{4} + \frac{\pi^4}{16} \qquad \bar{C}_5 = 5\left(\frac{7}{9} - \frac{7\pi^2}{9} + \frac{\pi^4}{16}\right). \tag{B.6}$$

We can then write the expression for the magnetization to order h^3 in the form

$$\frac{\pi\Delta M(h)}{g\mu_B h} = \sum_{n=0} C_n u^n - \frac{h^2}{3\Delta^2}\sum_{n=0} A_n u^n \tag{B.7}$$

where $A_n = 3(C_{n+1} - \bar{C}_{n+1})/2$ for $n \geqslant 0$. The coefficients of the terms in the second series to order u^4 are $A_0 = 1$, $A_1 = 4$ and

$$A_2 = \frac{65}{3} - \frac{3\pi^2}{2} \qquad A_3 = 15\left(\frac{280}{27} - \pi^2\right) \qquad A_4 = 15\left(\frac{847}{9} - \frac{91\pi^2}{9} + \frac{\pi^4}{16}\right). \tag{B.8}$$

In the Kondo limit the term proportional to $J_1(u)$ does not contribute to the h^3-coefficient, and it can be shown that the asymptotic contribution from the term proportional to $J_3(u)$ agrees with the result for the Kondo model (63) with T_K defined by

$$T_K = \Delta\sqrt{\frac{\pi u}{2}}\,e^{-\pi^2/8u + 1/2u}. \tag{B.9}$$

We can also use these results to deduce the terms in the renormalized perturbation calculations to higher orders. We will use this approach to find the fourth-order correction to our third-order result. We can deduce $\tilde{\Delta}$ and $\tilde{U}$ to fourth order in U from the Bethe *ansatz* results for γ and χ. These can be inverted to calculate the bare parameters U and Δ in terms of the renormalized ones to the same order in $\tilde{U}$. The results are

$$\frac{1}{\Delta} = \frac{1}{\tilde{\Delta}}\left(1 - \left(3 - \frac{\pi^2}{4}\right)\tilde{u}^2 - \left(24 + \frac{15\pi^2}{4} - \frac{5\pi^4}{8}\right)\tilde{u}^4 - \cdots\right) \tag{B.10}$$

$$u = \tilde{u}\left(1 - \left(12 - \frac{5\pi^2}{4}\right)\tilde{u}^3 + O(\tilde{u}^5)\right). \tag{B.11}$$

We can then use the results above for the h^3-term magnetization to fourth order in U, and rewrite them in terms of the renormalized parameters. In this way we calculate that the correction from the fourth-order terms to D', the H^3-coefficient in the Kondo limit, is -0.24145, which is 10% of the third-order contribution. As the coefficient in the Kondo regime has a factor $\sqrt{3}$, the exact result cannot be obtained within any finite-order renormalized perturbation calculation, as results to finite order in $\tilde{U}$ can be expressed as rational functions of the coefficients C_n and A_n, and these in turn are rational numbers and powers of π, which cannot generate to finite order the irrational number $\sqrt{3}$.

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