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# Non-equilibrium differential conductance through a quantum dot in a magnetic field

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#### **Abstract**

We derive an exact expression for the differential conductance for a quantum dot in an arbitrary magnetic field for small bias voltage. The derivation is based on the symmetric Anderson model using renormalized perturbation theory and is valid for all values of the on-site interaction U including the Kondo regime. We calculate the critical magnetic field for the splitting of the Kondo resonance to be seen in the differential conductivity as a function of bias voltage. Our calculations for small field show that the peak positions of the component resonances in the differential conductance are reduced substantially from estimates using the equilibrium Green function. We conclude that it is important to take the voltage dependence of the local retarded Green function into account in interpreting experimental results.

## 1. Introduction

Measurements of the temperature dependence of the differential conductance  $dI/dV_{ds}$  through a quantum dot in the linear response regime have been shown to be in good agreement with theoretical predictions based on magnetic impurity models [1, 2]. Measurements of  $dI/dV_{ds}$  through a quantum dot in the presence of an applied magnetic field, however, have revealed an apparent discrepancy between the magnetic splitting in the Kondo peaks deduced experimentally and theoretical predictions based on the same models [3–5]. The differential conductance measurements are made in the presence of a finite applied bias voltage  $V_{ds}$ , which is a situation for which there are few theoretical predictions. There are calculations based on the non-crossing approximation (NCA) [6]. This method, however, is known to break down in the Fermi liquid regime in the equilibrium case, so there is some uncertainty about the validity of the predictions in this case. There are also some recent perturbation calculations of Fuji and Uedo [7] using the Keldysh formalism, taking diagrams up to fourth order in the on-site interaction U into account. This approach should reliably describe the trends in the approach to the strong correlation limit, as the interaction strength is increased, but cannot fully describe the Kondo regime, where there is an exponential renormalization of the Kondo resonance width as a function of U. Rosch et al have calculated the differential conductance

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using a perturbative renormalization group calculation for the exchange coupling J to leading order in  $1/\ln(V_{ds}/T_{\rm K})$ , which is appropriate for the very high voltage regime ( $V_{ds} \gg T_{\rm K}$ ) [12] (see also [13]). This approach is, however, not suitable for investigating the Kondo regime, where  $V_{ds}$  and the magnetic field are of the order of the Kondo temperature  $T_{\rm K}$ .

More accurate methods [8–11] for the Kondo regime exist for calculations in an applied magnetic field, which have been used to interpret the experimental results [3–5], but they are restricted to the linear response (equilibrium) regime. It is not clear that using the equilibrium response for  $dI/dV_{ds}$  in the presence of an applied bias voltage will lead to reliable predictions. In this paper we examine the effect of a finite applied bias voltage in the small bias regime. In the limit of a small magnetic field B, we calculate asymptotically exactly the shifts of the peaks of the differential conductance of particular spin component for small, but finite  $V_{ds}$ . The results are based on renormalized perturbation theory and numerical renormalization group (NRG) calculations. We also deduce the value of the critical field  $B_c$  for two distinct peaks to be seen in  $dI/dV_{ds}$ . The knowledge of  $dI/dV_{ds}$  to order  $V_{ds}^2$  for arbitrary values of B is sufficient to determine  $B_c$  exactly.

In our treatment the quantum dot will be described by a single-impurity Anderson model with particle—hole symmetry coupled via left and right leads to two reservoirs of free electrons. The Anderson model has the form

$$H_{\rm AM} = \sum_{\sigma} \epsilon_{d\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{k,\sigma} (V_k d_{\sigma}^{\dagger} c_{k,\sigma} + V_k^* c_{k,\sigma}^{\dagger} d_{\sigma}) + \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^{\dagger} c_{k,\sigma}, \tag{1}$$

where  $\epsilon_{d\sigma} = \epsilon_d - \sigma g \mu_B B/2$  is the energy of the impurity levels with spin  $\sigma = \pm 1$  in a magnetic field B, U is the interaction at the impurity site, and  $V_k$  the hybridization matrix element to a band of conduction electrons with energy  $\epsilon_k$ . In the wide band limit the hybridization weighted density of states,  $\Delta(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k)$ , can be taken as a constant  $\Delta$ . Taking this limit justifies the neglect of any magnetic field term acting on the conduction electrons in (1) (Clogston–Anderson compensation theorem [14]). Any polarization of the conduction electrons only affects the impurity via the hybridization function  $\Delta(\omega)$  and any change to the conduction band density of states due to an applied magnetic field is only at the band edges  $(\pm D)$ , and hence negligible if  $g\mu_B B \ll D$ . Therefore, if  $\Delta(\omega)$  is independent of  $\omega$  the magnetic field does not need to be included in the electron band.

The single-impurity model can be applied to a quantum dot which is equally coupled via leads to left and right reservoirs. In this situation the charge on the quantum dot is coupled only to an even combination of states from the left and right channels by an effective hybridization  $V_k$ , so it can be mapped into a single-channel model. If there is a potential difference  $eV_{ds}$  due to a bias voltage  $V_{ds}$  ( $eV_{ds}$ ) is the electronic charge), then the chemical potentials in the left and right reservoirs differ from the average chemical potential  $\mu$  by  $eV_{ds}/2$  and  $-eV_{ds}/2$ , respectively.

A general expression for the current *I* due to the applied voltage through a quantum dot has been given by Hershfield *et al* [15] and Meir and Wingreen [16, 17], and specializing it to this symmetric case it takes the form

$$I = \frac{e\Delta}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \left[ f_{L}(\omega) - f_{R}(\omega) \right] \left[ -\operatorname{Im} G_{d\sigma}^{r}(\omega, V_{ds}) \right], \tag{2}$$

where  $G_d^{\rm r}(\omega,V_{ds})$  is the steady state retarded Green function on the dot site, and  $f_{\rm L}(\omega)$ ,  $f_{\rm R}(\omega)$  are Fermi distribution functions for the electrons in the left and right reservoirs, respectively, and h is Planck's constant.

The retarded Green function  $G_{d\sigma}^{r}(\omega, V_{ds})$  can be written in terms of a self-energy  $\Sigma_{\sigma}(\omega, V_{ds})$ ,

$$G_{d\sigma}^{r}(\omega, V_{ds}) = \frac{1}{\omega - \epsilon_d + i\Delta - \Sigma_{\sigma}(\omega, V_{ds})}.$$
(3)

Oguri [18, 19] has shown that this Green function for the symmetric model ( $\epsilon_d = -U/2$ ) in the Fermi liquid regime in the absence of a magnetic field to order  $\omega^2$  and  $(eV_{ds})^2$  can be expressed in the form

$$G_{d\sigma}^{r}(\omega, V_{ds}) = \frac{z}{\omega + i\tilde{\Delta} - \tilde{\Sigma}(\omega, V_{ds})}$$
(4)

where  $\tilde{\Sigma}(\omega, V_{ds})$  is a renormalized self-energy [20] given by

$$\tilde{\Sigma}(\omega, V_{ds}) = -ic \left[ \omega^2 + \frac{3}{4} (eV_{ds})^2 \right], \quad \text{with } c = \frac{1}{2\tilde{\Delta}} \left( \frac{\tilde{U}}{\pi \tilde{\Delta}} \right)^2$$
 (5)

expressed in terms of the renormalized parameters  $\tilde{\Delta}$  and  $\tilde{U}$ . These parameters [20] are defined in terms of the local impurity self-energy  $\Sigma(\omega)$  and local irreducible four-vertex  $\Gamma_{\uparrow\downarrow}(\omega_1,\omega_2,\omega_3,\omega_4)$  [20] for  $V_{ds}=0$ ,

$$\tilde{\Delta} = z\Delta, \qquad \tilde{U} = z^2 \Gamma_{\uparrow\downarrow}(0, 0, 0, 0),$$
(6)

where z is given by  $z = 1/(1 - \Sigma'(0))$ . The renormalized parameters  $\tilde{\Delta}$  and  $\tilde{U}$  can be calculated directly from NRG calculations, as described in [22, 23], where they are given in terms of the 'bare' parameters of the model  $\Delta$  and U. Alternatively they can also be deduced from the Bethe ansatz results [20].

We can generalize this result by including a magnetic field term [23, 24] to lowest order in B, and then  $G^{\rm r}_{d\sigma}(\omega)$  takes the form

$$G_{d\sigma}^{r}(\omega) = \frac{z}{\omega + \sigma \tilde{\eta}b + i\tilde{\Delta} - \tilde{\Sigma}_{\sigma}(\omega, V_{ds})},$$
(7)

where  $\sigma=\pm 1$ ,  $b=g\mu_B B/2$ , and  $\tilde{\eta}$  is a renormalization parameter defined as  $\tilde{\eta}(b)=z(b)(1-\Sigma_{\uparrow}(0,b)/b)$ . This renormalized parameter can be deduced from NRG calculations as shown in [23]<sup>3</sup>. We give an example in the Kondo regime for  $U/\pi\Delta=4$  in figure 1, where the ratio of the parameters to their values in zero field are plotted as a function of  $\log(b/T_{\rm K})$ . As  $b\to 0$ ,  $\tilde{\eta}(b)$  is independent of b such that  $\tilde{\eta}(b)\to R$ , where R is the Wilson or ' $\chi/\gamma$ ' ratio for zero magnetic field. In terms of the renormalized parameters for finite field, R(b) is given by  $R(b)=1+\tilde{U}(b)\tilde{\rho}_d^0(0,b)$  [20, 22], where the free quasiparticle density of states  $\tilde{\rho}_{d,\sigma}^0(\omega,b)$  is given by

$$\tilde{\rho}_{d,\sigma}^{0}(\omega,b) = \frac{\tilde{\Delta}(b)/\pi}{(\omega + \sigma b\tilde{\eta}(b))^{2} + \tilde{\Delta}^{2}(b)},$$
(8)

which is independent of the spin index  $\sigma$  for  $\omega = 0$ . There are in general  $B^2$  and higher order terms in the self-energy but for the moment we work only to first order in B so the renormalized self-energy  $\tilde{\Sigma}_{\sigma}(\omega, V_{ds})$  is still given by equation (5) with

$$c = c(b) = \frac{\pi \tilde{U}^2(b) [\tilde{\rho}_d^0(0, b)]^3}{2},\tag{9}$$

which reduces to (5) for  $b \to 0$ .

# 2. Weak field limit

We look at the effects of the different contributions to  $dI/dV_{ds}$  in turn. We consider the simplest situation to begin with and ignore the renormalized self-energy term in (7). The differential conductance (2) at T=0 then takes the form

$$\frac{\mathrm{d}I}{\mathrm{d}V_{ds}} = \frac{e^2}{h} \sum_{\nu} \frac{\tilde{\Delta}^2}{(eV_{ds}/2 - \nu\tilde{\eta}b)^2 + \tilde{\Delta}^2},\tag{10}$$

<sup>&</sup>lt;sup>3</sup>  $\tilde{\eta}$  corresponds to the ratio  $\tilde{\epsilon}_d(h)/h$  in [23].

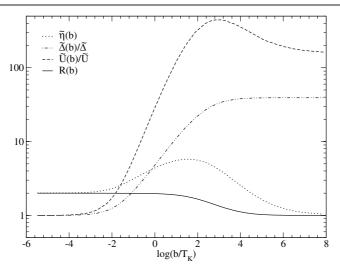


Figure 1. b dependence of the renormalized parameters for strong coupling  $(U/\pi \Delta = 4)$ , in relation with their b=0 values,  $\tilde{U}=\pi \tilde{\Delta}=4T_{\rm K}=0.0817\Delta$ . Note the logarithmic scale of the y-axis.

where  $\nu=\pm 1$ . The total result is expressed as a sum over  $\nu=\pm 1$ , rather than as a sum over  $\sigma=\pm 1$ , as both spin up and spin down states contribute to each resonance. Note that the result does not simply correspond to the non-interacting case, as it includes the many-body renormalization factor  $\tilde{\eta}$ . It corresponds to the case in which the interaction between the renormalized quasiparticles  $(\tilde{U})$  is neglected. In the Kondo regime  $\tilde{\eta}=2$ , so the effective Zeeman splitting of the resonance in this limit is twice the Zeeman splitting (2b) for non-interacting electrons (U=0). Note that the energy level on the dot is at the average chemical potential  $\mu$ , which is shifted by  $eV_{ds}/2$  with respect to the value at zero bias. The individual terms in (10) for each  $\nu$  have maxima at  $\pm 2\tilde{\eta}b$ . The maxima of the sum in general occur at a shifted position  $eV_{ds}^{\pm}=\pm 2\tilde{\eta}bf_{c}(\tilde{\eta}b,\tilde{\Delta})$  with

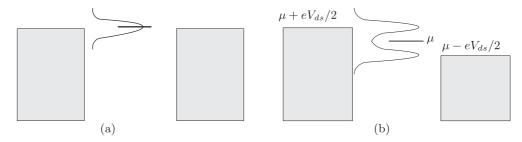
$$f_{c}(\tilde{\eta}b,\tilde{\Delta}) = \left[1 - \left(1 - \left[1 + (\tilde{\Delta}/\tilde{\eta}b)^{2}\right]^{1/2}\right)^{2}\right]^{1/2},\tag{11}$$

provided that  $\tilde{\eta}b > \tilde{\Delta}/\sqrt{3}$ . For  $\tilde{\eta}b \gg \tilde{\Delta}$  it can be approximated by  $f_{\rm c}(\tilde{\eta}b,\tilde{\Delta}) \simeq 1 - \frac{1}{8}\frac{\tilde{\Delta}^4}{(\tilde{\eta}b)^4}$ . The peak splitting is therefore  $e(V_{ds}^+ - V_{ds}^-) = 4\tilde{\eta}bf_{\rm c}(\tilde{\eta}b,\tilde{\Delta})$ . A maximum of the differential conductance, therefore, occurs when one of the quasiparticle peaks is coincident with left Fermi level at  $\mu + eV_{ds}/2$  and at the same time the other peak coincides with the right Fermi level,  $\mu - eV_{ds}/2$ . This is illustrated in figure 2. In the interpretation of the experimental results of  $dI/dV_{ds}$  the splitting of the Kondo resonance  $\Delta_{\rm Kondo}$  was identified with the voltage splitting  $e(V_{ds}^+ - V_{ds}^-) = \Delta_{\rm Kondo}$  [4, 5]. However, for the renormalized quasiparticles the Kondo splitting is  $\Delta_{\rm Kondo} = 2\tilde{\eta}b$ , which substituted in the above result gives  $e(V_{ds}^+ - V_{ds}^-) = 2\Delta_{\rm Kondo}$ . The factor of two difference is due to the many-body shift in the energy level on the dot, which was not taken into account in the interpretation of the experimental results in [4, 5].

We should also take into account the terms in the renormalized self-energy  $\tilde{\Sigma}(\omega, V_{ds})$ . For the moment we ignore the  $V_{ds}$  dependence of  $\tilde{\Sigma}(\omega, V_{ds})$ , and then

$$\frac{\mathrm{d}I}{\mathrm{d}V_{ds}} = \frac{e^2 \tilde{\Delta}}{h} \sum_{\nu} \frac{\tilde{\Delta} - \tilde{\Sigma}^I(\omega)}{(\omega - \nu \tilde{\eta}b)^2 + (\tilde{\Delta} - \tilde{\Sigma}^I(\omega))^2} \bigg|_{\omega = eV_{ds}/2},\tag{12}$$

where  $\tilde{\Sigma}^I(\omega, V_{ds})$  is the imaginary part of  $\tilde{\Sigma}(\omega, V_{ds})$  as given in equation (5). If the component spectral densities  $(\nu \pm 1)$  have maxima at  $\omega_{\pm}$  then this expression has maxima as a function



**Figure 2.** A schematic plot of the spectrum on the dot and chemical potentials for left/right lead  $(\mu \pm eV/2)$  and dot  $(\mu)$  for (a) zero bias and zero magnetic field and (b) finite voltage and finite field

of  $V_{ds}$  for  $2\omega_{\pm}$ . Working to lowest order in b, we find from the exact result for the self-energy to order  $\omega^2$  that for a maximum

$$\omega = \pm \tilde{\eta}b + \frac{\tilde{\Delta}}{2} \frac{\partial \tilde{\Sigma}^{I}}{\partial \omega} = \pm \tilde{\eta}b - \omega \tilde{\Delta}c(b). \tag{13}$$

The peak position in the resonances in the spectral density to first order in b is given by

$$\omega_{\pm} = \frac{\pm \tilde{\eta}b}{1 + \tilde{\Delta}c(b)}.\tag{14}$$

For  $b\to 0$  find  $\tilde\Delta c(b)\to \frac12(\frac{\tilde U}{\pi\tilde\Delta})^2=\frac12(R-1)^2$  and so this result corresponds to that of Logan and Dickens [9], and as derived from the renormalized perturbation calculations [21]. It shows that the effective Zeeman splitting of the free quasiparticles,  $2\tilde\eta b$ , is reduced in the spectral densities by a factor arising from the  $\omega^2$  term in the imaginary part of the self-energy. In the Kondo limit,  $\tilde U=\pi\tilde\Delta=4T_{\rm K}$ , so  $\tilde U/\pi\tilde\Delta=1$  and  $\tilde\eta=R=2$ ; hence the peak position of 2b is reduced by a factor of two-thirds. This effect will be reflected in the voltage difference between the differential conductance peaks,

$$e(V_{ds}^{+} - V_{ds}^{-}) = \frac{4\tilde{\eta}b}{1 + \tilde{\Lambda}c(b)} f_{c}(\tilde{\eta}b, \tilde{\Delta}), \tag{15}$$

where  $f_c$  is a correction factor due to the overlap of resonances similar to the above, which can be computed numerically. However, in calculating this voltage difference we cannot neglect the voltage dependence of the self-energy.

When we take the  $V_{ds}$  dependence of the retarded Green function into account,

$$\frac{\mathrm{d}I}{\mathrm{d}V_{ds}} = -\frac{e^2\Delta}{h} \sum_{\sigma} \operatorname{Im} G_{d\sigma}^{\mathrm{r}}(eV_{ds}/2, V_{ds}) + \frac{2e\Delta}{h} \sum_{\sigma} \int_{0}^{eV_{ds}/2} \mathrm{d}\omega \left[ -\operatorname{Im} \frac{\partial G_{d,\sigma}(\omega, V_{ds})}{\partial V_{ds}} \right]. \tag{16}$$

In considering the contribution from the first term on the right-hand side we can replace the  $eV_{ds}$  in the self-energy by  $2\omega$ , and then see where it has a maximum as a function of  $\omega$ . This will correspond to the calculation we have just done except that the  $\omega^2$  term in  $\tilde{\Sigma}_I(\omega)$  will have an extra factor of four, as we can see from equation (5). We get the modified result,

$$e(V_{ds}^{+} - V_{ds}^{-}) = \frac{4\tilde{\eta}b}{1 + 4\tilde{\Delta}c(b)} f_{c}(\tilde{\eta}b, \tilde{\Delta}). \tag{17}$$

In the Kondo regime and for  $b \to 0$  the reduction factor arising from the self-energy including the voltage dependence is now one-third, so the splitting on including this term is reduced by an extra factor of two when the voltage dependence in the retarded Green function is taken

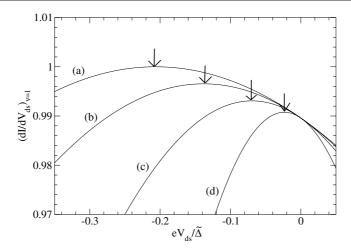


Figure 3. The shift of the component resonance ( $\nu = 1$ ) in the differential conductance (units of  $e^2/h$ ) in a magnetic field for  $b/\tilde{\Delta} = 0.05$  as a function of the bias voltage  $eV_{ds}/\tilde{\Delta}$ , according to the inclusion of different contributions as described in the text. The arrows indicate the respective maxima.

into account. We do need to take account, however, of the second term on the right-hand side of equation (16) involving an integral over  $\omega$ . This term can be written as

$$\frac{3c(b)e^{2}}{h}V_{ds}\tilde{\Delta}\sum_{v}\int_{0}^{eV_{ds}/2}d\omega\frac{(\omega+v\tilde{\eta}b)^{2}-(\tilde{\Delta}+c(b)(\omega^{2}+3(eV_{ds})^{2}/4))^{2}}{[(\omega+v\tilde{\eta}b)^{2}+(\tilde{\Delta}+c(b)(\omega^{2}+3(eV_{ds})^{2}/4))^{2}]^{2}}.$$
(18)

If we plot all the contributions to  $\mathrm{d}I/\mathrm{d}V_{ds}$  in the very weak field regime then, due to overlap, no magnetic field splitting can be observed. We can calculate, however, the shifts in the component resonance for  $\nu=\pm 1$ . In figure 3 we plot the terms in the differential conductance (in units of  $e^2/h$ ) given by equation (16) as a function of  $eV_{ds}/\tilde{\Delta}$ , where we use  $\nu=1$  in (12) for the first term in (16) and (18) for the second term in (16). We take values corresponding to the Kondo regime, with  $R=\tilde{\eta}=2$ ,  $b/\tilde{\Delta}=0.05$  ( $\pi\tilde{\Delta}=4T_{\rm K}$ ). We have distinguished between the different contributions: (a) is the case for the non-interacting quasiparticles, (b) includes the  $\omega^2$  term in the renormalized self-energy, (c) includes the first term in equation (16), and (d) takes into account the full expression including the integral term in (18). We see that the integral term arising from the voltage dependence of  $G_{d,\sigma}(\omega,V_{ds})$  causes a significant further reduction of the magnetic shift beyond that estimated from the first term in equation (16). In an experimental conductance measurement this is not observable, however, due to the overlap of the two components.

## 3. Critical field

Our derivation is restricted to the regime where  $eV_{ds}$  is small compared to  $\tilde{\Delta}$ . These results are sufficient for us to deduce the critical value of the magnetic field  $b_c$  at which two distinct peaks begin to appear in the total differential response. For values of  $b < b_c$  the differential conductance will have a maximum at  $V_{ds} = 0$ , and for  $b > b_c$  this will become a minimum. From the coefficient of  $dI/dV_{ds}$  to order  $V_{ds}^2$  we can determine the point at which it changes sign as a function of b, and hence determine  $b_c$ . The contribution from the integral term in equation (18) to order  $V_{ds}^2$  can be evaluated trivially, as it is sufficient to this order to put

 $\omega = V_{ds} = 0$  in the integrand. As a first estimate using the above results the value of  $b_c$  can be calculated analytically, and the result expressed entirely in terms of  $\tilde{\Delta}$  and the Wilson ratio  $R = \eta(0) = 1 + \tilde{U}/\pi \tilde{\Delta}$ ,

$$\frac{b_{\rm c}^2}{\tilde{\Lambda}^2} = \frac{\sqrt{9 + 20(R - 1)^2 (1 + 5(R - 1)^2)} - 3}{10R^2 (R - 1)^2}.$$
 (19)

In the non-interacting case, R=1 and  $b_c/\Delta=1/\sqrt{3}=0.577$ , which corresponds to  $f_c(\tilde{\eta}b,\tilde{\Delta})=0$  from equation (11), and in the Kondo regime, R=2,  $\tilde{\Delta}=4T_K/\pi$ , and  $b_c/T_K=0.582$ , with  $T_K$  given by

$$T_{\rm K} = \Delta \left(\frac{U}{2\Delta}\right)^{1/2} e^{-\pi U/8\Delta + \pi \Delta/2U}.$$
 (20)

If the  $V_{ds}$  dependence of the Green function is neglected the result in the Kondo regime is  $b_c/T_K = 0.491$ : significantly smaller than if this term is included.

The estimated critical magnetic field is comparable with  $\tilde{\Delta}$ , and for  $U \neq 0$  it may not be sufficient to work to linear order in B. It is possible to work with an arbitrary magnetic field, but in this case the renormalized parameters become field dependent. The renormalized self-energy to order  $\omega^2$  and  $V_{ds}^2$  can be expressed in the form

$$\tilde{\Sigma}_{\sigma}(\omega, V_{ds}) = -c(b) \left[ i \left( \omega^2 + 3 \left( \frac{eV_{ds}}{2} \right)^2 \right) + \frac{\sigma b \tilde{\eta}(b)}{\tilde{\Delta}(b)} \left( \alpha_{\omega}(b) \omega^2 + \alpha_V(b) \left( \frac{eV_{ds}}{2} \right)^2 \right) \right], \tag{21}$$

where c(b) is given in equation (9). The coefficients for the expansion of the real part of  $\tilde{\Sigma}_{\sigma}(\omega, V_{ds})$  are

$$\alpha_{\omega}(b) = 2 + \frac{2I(b)\tilde{\Delta}(b)}{\tilde{\epsilon}(b)[\tilde{\rho}_{J}^{0}(0,b)]^{2}},\tag{22}$$

where  $\tilde{\xi}(b) = \pi \, \tilde{\rho}_d^0(0, b) \tilde{\eta}(b) b$  and I(b) is the integral

$$I(b) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G_{\downarrow}^{0}(\omega'') G_{\downarrow}^{0}(\omega'' + \omega') [G_{\uparrow}^{0}(\omega')]^{3} \frac{\mathrm{d}\omega''}{2\pi} \frac{\mathrm{d}\omega'}{2\pi},\tag{23}$$

where  $[G^0_\sigma(\omega)]^{-1} = \omega + \sigma \tilde{\eta} b + i \tilde{\Delta} \mathrm{sgn}(\omega)$  is the renormalized free propagator for T=0.  $\alpha_\omega(b)$  is obtained from the second order derivative of the renormalized self-energy evaluated at  $\omega=0$  using the renormalized perturbation theory to order  $\tilde{U}^2$ . This reduces to the exact result of Yamada [26] for the symmetric model for b=0. The corresponding coefficient  $\alpha_V(b)$  for finite voltage is calculated from the  $\tilde{U}^2$  contribution to the retarded self-energy in the Keldysh formalism [25], where the propagator  $G^{--}_{0,\sigma}(\omega,V_{ds})$  taken to order  $V^2_{ds}$  for T=0 is

$$G_{0,\sigma}^{--}(\omega, V_{ds}) = G_{\sigma}^{0}(\omega) - \frac{i\tilde{\Delta}\delta'(\omega)(eV_{ds})^{2}/4}{(\omega - \sigma\tilde{\eta}b)^{2} + \tilde{\Delta}^{2}},$$
(24)

where  $\delta'(\omega)$  is the derivative of the delta-function, together with a similar equation for  $G_{0,\sigma}^{+-}(\omega,V_{ds})$ . The result for  $\tilde{\alpha}(b)$  is

$$\tilde{\alpha}_{V}(b) = 1 + \frac{\tilde{\Delta}(b)}{2\tilde{\xi}(h)\tilde{\eta}(b)b} \left[ 1 - \frac{\tilde{\eta}(b)b}{\tilde{\Delta}(b)} \tan^{-1} \left( \frac{\tilde{\eta}(b)b}{\tilde{\Delta}(b)} \right) \left( 4 + \frac{\tilde{\Delta}(b)}{\tilde{\xi}(h)\tilde{\eta}(b)b} \right) \right]. \tag{25}$$

The contribution to the real part of the self-energy to order  $\omega^2$  and  $V_{ds}^2$  is proportional to  $\sigma \tilde{\eta}(b)b$ . It might be thought that such a term should cancel out in taking the sum over the two

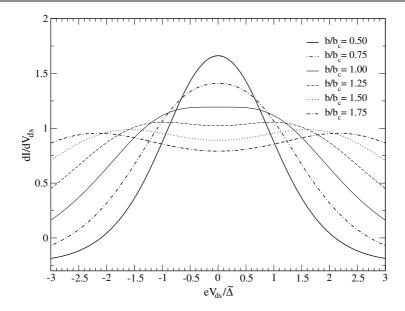


Figure 4. The total differential conductance (in units of  $e^2/h$ ) in the Kondo regime for larger magnetic field values, calculated using equation (16) taking into account the full self-energy expansion from (21). These results are asymptotically exact for  $eV_{ds}/\tilde{\Delta} \ll 1$  and approximate, based on a second order expansion in  $eV_{ds}$  for larger values.

spin components. However, there is a  $\sigma$ -independent contribution from a cross term with the effective Zeeman term  $\sigma b \eta(b)$ , which has to be included. In the limit  $b \to 0$  equation (21) reduces to (5).

The equation for the critical field  $b_{\rm c}$  becomes

$$\frac{b^2}{\tilde{\Delta}^2(b)} = \frac{\sqrt{(3 - \alpha(b)\gamma(b))^2 + 4\gamma(b)(5 - \alpha(b))(1 + 5\gamma(b))} - 3 + \alpha(b)\gamma(b)}{2\gamma(b)(5 - \alpha(b))\tilde{\eta}(b)^2}$$
(26)

where  $\alpha(b) = \alpha_{\omega}(b) + \alpha_{V}(b)$ , and

$$\gamma(b) = \pi \tilde{\Delta}(b)\tilde{U}^{2}(b)[\tilde{\rho}_{d}^{0}(0,b)]^{3} = \pi \tilde{\Delta}(b)\tilde{\rho}_{d}^{0}(0,b)(R(b)-1)^{2}. \tag{27}$$

Equation (26) is an implicit equation for  $b_c$  which can be solved by iteration starting from the much simpler result (19), obtained within the linear approximation.

For a strong coupling situation  $(U/\pi\Delta=4)$  the result for the critical field obtained by iterating equation (26) and using the b-dependent renormalized parameters taken from figure 1 is  $b_c \simeq 0.459\tilde{\Delta} = 0.584T_K$ . This differs only by 0.3% from the value obtained from (19). The small difference is due to the fact that the various correction terms due to the b dependence of the parameters in the more general formula (26) tend to cancel, giving only a small resultant change.

Plots of the total differential conductance for various fields above and below the critical field are displayed in figure 4. We have taken the full self-energy as given in (21) into account, including the field dependence of the renormalized parameters. Our results are asymptotically exact only for small  $V_{ds}$  and a more complete theory is required to calculate the splitting at larger bias voltages. The major problem to be solved is the dependence of the self-energy on the voltage bias term, when  $eV_{ds}$  is comparable with and greater than the Kondo temperature  $T_{\rm K}$ , so that a detailed comparison with experiment can be made with the experimental results in this regime.

#### 4. Conclusions

Measurements of the differential conductance in a magnetic field have been used to infer the magnitude of the magnetic splitting of a Kondo resonance [4, 5]. The results reveal an apparent disagreement with theoretical predictions, but the comparisons with theory have been based on calculations of the equilibrium Green function for the dot. It is not clear that this will constitute a reasonable approximation at the finite bias voltages used in the experiment. To examine this question we have derived an expression for the differential conductivity through a quantum dot, described by a symmetric Anderson model, for small bias voltages and arbitrary magnetic field. This has enabled us to estimate the effect of the voltage dependent terms from the non-equilibrium dot Green function. Our estimates of the shifts of the component resonances for small magnetic field values differ significantly from the values obtained using the equilibrium Green function. We conclude that it is important to take this voltage dependence into account and use the non-equilibrium Green function for a meaningful comparison with experiment.

Though our calculations are restricted to the small voltage regime we have also been able to estimate the value of the critical field  $B_{\rm c}$  for the emergence of two distinct peaks in the total differential conductance. Our approach is applicable in all ranges of the interaction U from the weak coupling to the strong coupling Kondo regime for T=0. They complement the perturbation calculations in U of Fuji and Ueda [7] for the same model. It is difficult to make a comparison with their results, however, because the interaction simultaneously modifies the renormalized parameters, such as  $\tilde{\eta}(b)$ , and introduces a dependence on  $V_{ds}$ , both directly and through the  $\omega$  dependence in the self-energy. These three effects of the interaction can be clearly distinguished within our formulation and taken separately into account. It should be possible to extend our calculations to larger values of  $V_{ds}$  using a renormalized version of the perturbation theory, and this approach is currently being investigated.

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