NONEQUILIBRIUM ELECTRON TRANSPORT THROUGH NANOSTRUCTURES: CORRELATION EFFECTS

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Abstract. We consider electron transport through a quantum dot in the Coulomb blockade regime, when the dot has a total spin $\frac{1}{2}$. The low energy physics of this system is modeled by a Kondo-type hamiltonian describing spin-dependent tunneling and exchange interaction of the electron spins in the leads and the local spin. We show that in the regime of large transport voltage V and magnetic field B with $\max(V, B) \gg T_K$, where T_K is the Kondo temperature, renormalized perturbation theory is valid. Physical quantities such as the differential conductance G and the local magnetization M may be calculated in a controlled way by summing the leading logarithmic terms in each order of perturbation theory. We develop a poor man's scaling renormalization group treatment for frequency dependent coupling functions, which allows to calculate G and M to leading order in $1/\ell n[(V, B)/T_K]$.

1. Introduction

The transport of electrons through a quantum dot in the limit of weak coupling to the leads is dominated by Coulomb interaction effects, forcing integral electron charge on the dot (1) (Coulomb blockade). In the case that the total spin of the dot is nonzero, however, the antiferromagnetic exchange interaction of this local spin with the conduction electron spins in the leads gives rise to a Kondo resonance in the local density of states at the Fermi level. Electron transport may then take place via resonance tunneling, thus removing the Coulomb blockade (2, 3). This has been seen in a number of experiments (4, 5, 6, 7, 8).

Powerful methods have been developed to describe this strong coupling problem, among them methods based on the renormalization group idea, in a simplified form (9) ("poor man's scaling") and in a full numerical implementation by Wilson (10), exact methods for calculating the thermodynamic quantities using the Bethe ansatz (11), conformal field theory (12) and resummations of perturbation theory using auxiliary particle representations (13) to access dynamical quantities.

Necessary prerequisites for the existence of the Kondo effect are (i) the spin degeneracy of the ground state of the quantum dot, and (ii) quantum coherence over sufficiently long time periods. The characteristic energy scale against perturbations have to be measured is the Kondo temperature $T_K \simeq D\sqrt{JN_0}\exp(-\frac{1}{2N_0 J})$, where J is the exchange coupling constant, N_0 is the conduction electron density of states per spin at the Fermi level and D is the conduction band width.

Nonlinear transport through a Kondo system has been considered by several authors. Early on, Appelbaum (15) calculated the differential conductance $G(V, B)$ for large bias voltage V in a finite magnetic field B, assuming erroneously, however, that the local spin remains in thermal equilibrium. König et al. (16) calculated $G(V, B)$ for an Anderson model, employing a certain resummation of perturbation theory. Brief accounts of the work to be presented below have been published elsewhere (14, 17).

2. Magnetization and Conductance in Perturbation Theory

We study the following Kondo-type model Hamiltonian of a quantum dot:

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma,\alpha=L,R} (\varepsilon_{\mathbf{k}} - \mu_\alpha) c^\dagger_{\alpha\mathbf{k}\sigma} c_{\alpha\mathbf{k}\sigma} - BS_z \\ &\quad + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma',\alpha,\alpha'=L,R} J_{\alpha'\alpha}\, \mathbf{S} \cdot (c^\dagger_{\alpha'\mathbf{k}'\sigma'} \tau_{\sigma'\sigma} c_{\alpha\mathbf{k}\sigma}), \end{aligned} \tag{1}$$

where $\mathbf{S}$ is the local spin operator on the dot (assumed to be $S = \frac{1}{2}$) and τ is the vector of Pauli matrices. The $c^+_{\alpha\mathbf{k}\sigma}$ create conduction electrons with momentum $\mathbf{k}$ and spin σ in lead α. The chemical potential shifts induced by the bias voltage are given by $\mu_{L,R} = \pm V/2$ for the left (L) and right (R) lead. The exchange energies $J_{\alpha\alpha'}$, $\alpha = L, R$, will be assumed to have the symmetry $J_{RR} = J_{LL}$ and $J_{LR} = J_{RL}$. We shall use the dimensionless coupling constants $g_d = N_0 J_{RR}$ and $g_{LR} = N_0 J_{LR}$, with N_0 the local density of states at the Fermi energy, assumed to be flat in the accessible regime $\mid \omega \mid \leq V, B$. A magnetic field is included, inducing a Zeeman splitting of the magnetic levels of the local spin $\omega_\gamma = -\gamma B/2$, $\gamma = \pm 1$. The effect of the magnetic field on the conduction electrons gives only rise to particle-hole asymmetry terms, which are usually small and may be neglected.

In lowest order perturbation theory the current through the dot is given by the Golden Rule expression

$$I = \frac{\pi e}{4\hbar}\int d\omega \sum_{\gamma=\pm 1} n_\gamma \Big[g_1^2 f_{\omega-\mu_L}(1-f_{\omega-\mu_R}) + 2g_2^2 f_{\omega-\mu_L}(1-f_{\omega-\mu_R-\gamma B})\Big] - (L \leftrightarrow R) \qquad (2)$$

where g_1 and g_2 are the bare dimensionless coupling constants for spin-nonflip and spin-flip interaction, $g_1 = g_2 = N_0 J_{LR}$, $f_{\omega-\mu_\alpha}$ is the Fermi function in the lead $\alpha = L, R$, and γB is the Zeeman energy transfer taking place in a spin flip process. At low temperatures, $T \ll V, B$, the product of Fermi functions limits the energy integration to the window $\mu_R < \omega < \mu_L$ and $\mu_R + \gamma B < \omega < \mu_L$, respectively. The current is seen to depend on the occupation $n_\gamma = \frac{1}{2}(1+\gamma M)$ of the local spin states, where M is the magnetization.

For sufficiently small voltage, $V \ll T$, the local spin system is in thermal equilibrium. In the opposite limit, $V \gg T$, the stationary current through the dot drives the system out of equilibrium. The occupation numbers n_γ are then determined by the rate equation $\frac{\partial}{\partial t} n_\gamma = C_\gamma\{n_{\gamma'}\} = 0$, where C is the collision integral. This leads to the condition (assuming $J_{LR} = J_{LL}$ here)

$$n_\uparrow \sum_{\alpha,\alpha'=L,R} \int d\omega g_2^2 f_{\omega-\mu_\alpha}\Big(1 - f_{\omega-\mu_{\alpha'}-B}\Big) = = n_\downarrow \sum_{\alpha,\alpha'=L,R} \int d\omega g_2^2 f_{\omega-\mu_\alpha}\Big(1 - f_{\omega-\mu_{\alpha'}+B}\Big) \,. \qquad (3)$$

The spin-flip coupling constant g_2 cancels out of this equation, yielding the nonequilibrium magnetization as given by (5) in the limit $J \to 0$,

In the limit $V \to 0$, the equilibrium result $M = \tanh \frac{B}{2T}$ is recovered, whereas in the limit $V \gg B, T$, $M = \frac{2B}{V}$, independent of temperature. This result has been obtained independently in (18, 20).

In order to calculate higher order contributions in perturbation theory in J we switch now to a more formal description in terms of nonequilibrium Green's functions. We find it convenient to represent the local spin operator in pseudo fermion (PF) language (19), $\mathbf{S} = \frac{1}{2}\sum_{\gamma\gamma'} f_\gamma^+ \tau_{\gamma\gamma'} f_{\gamma'}$, where f_γ^+ creates a pseudofermion of spin $\gamma = \uparrow, \downarrow$ at the dot. The projection onto the physical sector of Hilbert space, with pseudofermion occupation number $Q = \sum_\gamma f_\gamma^+ f_\gamma = 1$, is done by adding a term λQ to the Hamiltonian and taking the limit $\lambda \to \infty$. This means that the PF system is taken in the low density limit. The Feynman diagrams of perturbation theory in the exchange interaction will therefore have one PF loop at most.

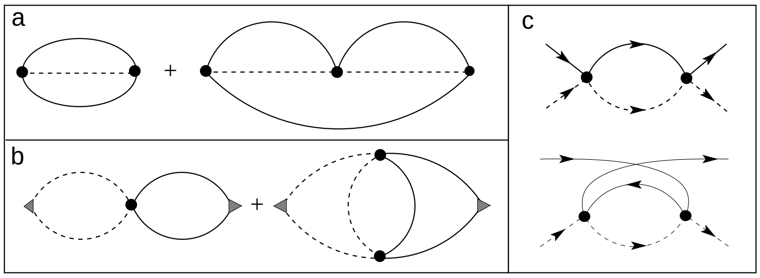

Figure 1. Feynman diagrams for (a) PF self-energies, (b) current and (c) vertices entering the 1-loop RG equation. PF (electron-) propagators are displayed as dashed (full) lines.

The local magnetization can be calculated in terms of the PF Green's function $G^<_\gamma(\omega)$ as $M = \sum_{\gamma=\pm 1} \gamma \int \frac{d\omega}{2\pi i} G^<_\gamma(\omega)$, where $G^<$ is found by solving a quantum kinetic equation. In steady state one finds

$$G^<_\gamma(\omega)\Gamma_\gamma(\omega) = \Sigma^<_\gamma(\omega) A_\gamma(\omega) \tag{4}$$

where $A_\gamma(\omega)$ is the PF spectral function, $\Sigma^<_\gamma(\omega)$ is the lesser component of the self-energy and $\Gamma_\gamma(\omega)$ its imaginary part. In general Eq. (4) is an integral equation for $G^<_\gamma(\omega) = in_\gamma(\omega)A_\gamma(\omega)$, which, however, can be approximated in a controlled way by making use of the sharply peaked form of $A_\gamma(\omega)$ to give an algebraic equation for $n_\gamma(0)$. In this form Eq. (4) corresponds to the rate equation discussed above, with higher order processes included in the transition amplitudes. The diagrams of the self-energy up to third order in J are depicted in Fig. 1a. Note that the lines represent Keldysh matrix Green's functions dressed with arrows in all topologically different ways. The result including leading logarithmic corrections is found as

$$M = \frac{Z}{\coth \frac{B}{2T}\left[\frac{Z}{2} + g_-^2 B(1+\mathcal{L}(B))\right] + g_{LR}^2(c(B)+c(-B))} \tag{5}$$

where

$$Z = 2g_+^2 B(1+\mathcal{L}(B)) + 2g_{LR}^2\Big[2B + (V+B)\mathcal{L}(V+B) - (V-B)\mathcal{L}(V-B)\Big] \tag{6}$$

and we use the abbreviations $g_\pm^2 = g_d^2 \pm g_{LR}^2$, $\mathcal{L}(B) = 2g_d \ell n \frac{D}{|B|}$, and $c(B) = \coth \frac{V+B}{2T}[(V+B)(1+\mathcal{L}(V+B)) + V\mathcal{L}(V) + B\mathcal{L}(B)]$. We note that logarithmic corrections of order $g^3 \ell n D$ to the self-energies lead to corrections of order $g \ell n D$ to M. These corrections are larger than the leading logarithmic corrections in equilibrium ($V \to 0$), which are of order $g^2 \ell n D$. A corresponding result of the current I is given in (17).

3. Resummation of Perturbation Theory in Nonequilibrium: a Poor Man's Scaling Approach

Even for small coupling constants g and for sufficiently large V and B, such that $V, B \gg T_K$, but still in the scaling regime $V, B \ll D$, such that $g\ell n(D/V) \ll 1$, bare perturbation theory converges slowly. It is necessary to sum the leading logarithmic contributions in all orders of PT. In the equilibrium state a powerful method is available to perform this resummation in a controlled way: the perturbative renormalization group method (9). It makes use of the fundamental idea that a change of the cut-off D can be fully absorbed into a redefinition of the coupling constant g. As long as the running coupling constant $g(D)$ is small, the change of g under an infinitesimal change of D, $\partial g/\partial \ell n D$, may be calculated in perturbation theory. It is well known that in the equilibrium Kondo problem the coupling constant is found to grow to infinity, thus leaving the perturbative regime beyond $g \sim 1$. A nonperturbative treatment is then necessary, as shown by Wilson (10) in his pioneering work on the numerical RG. In the nonequilibrium situation, the RG flow is cut-off by inelastic processes already within the weak coupling regime, such that perturbation theory is valid (14). This is true at least for the case $J_{LR} = J_{LL}, J_{RR}$, considered here. While the discussion of the RG flow in (14) was a qualitative one, motivated by results obtained in the so-called "Non-crossing approximation" for the Anderson model, and applied only to the limit $B = 0$, here we consider the RG formulation on a more fundamental level. A different and considerably more involved real-time RG scheme has been developed by Schoeller and König (21).

An analysis of the PT result Eq. (5) suggests that the frequency dependence of the couplings becomes important. In order to understand how these frequency dependencies are generated on the lowest level, i.e. in one-loop order, it is sufficient to analyze the behavior of the vertex corrections shown in Fig. 1c under a change of cut-off. Logarithmic corrections in perturbation theory are generated by PF - conduction electron bubbles containing the product of a real part of a PF Green's function, $1/(\omega \pm B/2)$, and the Keldysh component of the local conduction electron line, $-2\pi i N_0 \tanh[(\omega - \mu_\alpha)/2T]$. If the energy of the PF - conduction electron intermediate state is within the interval $[-D, D]$ the process will contribute to the renormalization of the coupling function $g(\omega)$, otherwise it will not. In general the coupling functions depend on three frequencies (taking energy conservation into account). Using the fact that the spectral function of the PFs is sharply peaked at $\omega = \mp B/2$, we set two of the three frequencies to $\omega = \mp B/2$, keeping only one frequency variable. In addition, the frequency dependence may be neglected within the running band-width, $|\ \omega\ | < D$. The spin structure of the general coupling functions is given by two invariant amplitudes, $\tilde{g}_2$ for spin flip and $\tilde{g}_1$ for spin non-flip processes

$$g^{\alpha\sigma,\omega;\alpha',\sigma',\omega-(\gamma-\gamma')B}_{\gamma,-\gamma B/2;\gamma',-\gamma' B/2} = \tau^z_{\sigma\sigma'}\tau^z_{\gamma\gamma'}\tilde{g}_1(\omega)+(\tau^x_{\sigma\sigma'}\tau^x_{\gamma\gamma'}+\tau^y_{\sigma\sigma'}\tau^y_{\gamma\gamma'})\tilde{g}_2(\omega-\gamma B/2) \quad (7)$$

where $g^{a;a'}_{b;b'}$ denotes the coupling function for conduction electrons of spin σ and energy ω in lead $\alpha (a = (\alpha, \sigma, \omega))$ interacting with a pseudo fermion in state $b = (\gamma, \omega_f)$ and going into states a', b'. The two frequency-dependent running coupling functions $\tilde{g}_1(\omega)$ and $\tilde{g}_2(\omega)$ obey the following flow equations,

$$\begin{aligned} \frac{\partial \tilde{g}_1(\omega)}{\partial \ln D} &= -\frac{1}{2}\sum_{\alpha=\pm 1} \tilde{g}_2^2(\frac{B+\alpha V}{2})\Big(\Theta_{\omega+B+\alpha\frac{V}{2}} + \Theta_{\omega-B-\alpha\frac{V}{2}}\Big) \\ \frac{\partial \tilde{g}_2(\omega)}{\partial \ell n D} &= -\frac{1}{2}\tilde{g}_1(\frac{V}{2})\sum_{\alpha=\pm 1} \tilde{g}_2(\frac{B+\alpha V}{2})\Big(\Theta_{\omega+\frac{B+\alpha V}{2}} + \Theta_{\omega-\frac{B+\alpha V}{2}}\Big) \end{aligned} \quad (8)$$

with initial condition $\tilde{g}_1(\omega) = \tilde{g}_2(\omega) = JN_0$ and $\Theta_\omega = \Theta(D- \mid \omega \mid)$. In the limit $V, B \to 0$, Eq. (8) reduces to the well-known scaling equations (6).

There is, however, still one additional effect missing: the finite relaxation of the spins even in the limit $T \to 0$ leading to inelastic broadening of the local spin levels, which we identify with the transverse spin relaxation rate $\Gamma = 1/T_2$. Within the PF representation this effect shows up as a finite imaginary part of the PF self-energy.

Assuming the RG flow to be stopped at the scale Γ, we replace the step functions Θ_ω in Eq. (8) by $\Theta(D - \sqrt{\omega^2+\Gamma^2})$. The decay rate Γ has to be calculated self-consistently with the solution of the flow equations (8). Starting from the golden rule expression for the transverse relaxation rate,

$$\begin{aligned} \Gamma &= \frac{\pi}{4\hbar}\sum_{\alpha,\alpha'=L,R,\gamma=\uparrow,\downarrow}\int d\omega \Big[\tilde{g}_1(\omega)^2 f_{\omega-\mu_\alpha}(1-f_{\omega-\mu_{\alpha'}}) \\ &\quad + \tilde{g}_2(\omega-\gamma B/2)^2 f_{\omega-\mu_\alpha}(1-f_{\omega-\mu_{\alpha'}-\gamma B})\Big] \end{aligned} \quad (9)$$

the renormalized Γ is obtained by replacing $g_{1,2}$ by $\tilde{g}_{1,2}(\omega)$ as determined from the solution of (2).

We are now ready to calculate further physical quantities. The renormalized value of the magnetization is obtained by substituting $\tilde{g}_{1,2}(\omega)$ in place of $g_{1,2}$ in the Golden Rule expression (3). In Fig. 2b we show the fully renormalized result for M as a function of V/B for different values of B.

The charge current I is calculated from Eq. (2) inserting the renormalized coupling functions. Fig. 2a shows a comparison of the differential

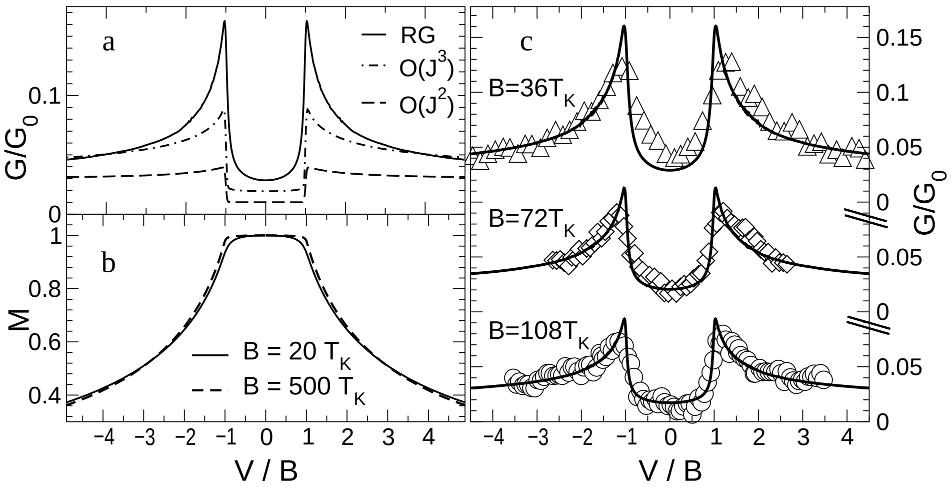

Figure 2. a) Conductance $G(V/B)$ calculated in leading (dashed line) and next-to-leading (dot-dashed line) order PT compared to the result of perturbative RG (solid line) for $B = 100T_K$, $D = 10^4 T_K$, $T_K = D\sqrt{g}e^{-1/2g}$). b) Local magnetization $M(V/B, B/T_K)$ of a symmetric dot for fixed magnetic field $B = 20, 500\, T_K$. c) Experiments by Ralph and Buhrman (22) (symbols) on transport through metallic point contacts in magnetic fields $0.85, 1.7, 2.55$ T ($B = 36, 72, 104\, T_K$ where $T_K \approx 30$mK (22)).

conductance $G(V) = dI/dV$ obtained in this way, with the bare result (2) and the PT result including leading logarithmic corrections.

The peak structures in $G(V, B)$ appearing at $V = \pm B$ have been detected in experiment. In order to reach large values of B/T_K, it is necessary to have relatively low T_K. This happened to be the case in transport through metallic point contacts, containing a magnetic impurity (22). In Fig. 2c the result of our theory using the value of $T_K \simeq 30mK$ given in (22) is compared to the experimental data, after subtracting a background contribution (see (17) for details). The agreement is seen to be excellent.

4. Conclusion

We considered the transport of electrons through a Kondo dot in the regime of large transport voltage V and in the presence of a magnetic field B, such that $\max(V, B) \gg T_K$ is satisfied. A finite difference of the chemical potentials in the two leads, $\mu_L - \mu_R = V$, changes the RG flow substantially. Furthermore, it opens an energy window for inelastic processes even at $T = 0$, leading to a broadening Γ of the spin sublevels of the dot and providing a cut-off for the scaling towards the Kondo fixed point. A finite magnetic field induces a local magnetization M at the dot, which for $V \gg T_K, T$ is independent of temperature, being solely controlled by the voltage V. We derived a set of RG equations within a poor man's scaling approximation, which for once reproduce the bare PT result, but then may be integrated to give the fully renormalized result. The integration is done including the self-consistently determined cut-off Γ. The results obtained in this way are valid up to corrections of order $1/\ell n[(V,B)/T_K]$.

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References

1. I. Aleiner, P. Brouwer, and L. Glazman, Phys. Rep. **358**, 309 (2002).
2. L. Glazman and M. Raikh, JETP Letters **47**, 452 (1988).
3. T. Ng and P.A. Lee, Phys. Rev. Lett. **61**, 1768 (1988).
4. D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav and M. Kastner, Nature **391**, 156 (1998).
5. S. Cronenwett, T. Oosterkamp and L. Kouwenhoven, Science **281**, 540 (1998).
6. J. Schmid, J. Weis, K. Eberl, and K. v. Klitzing, Physica B **258**, 182 (1998).
7. J. Nygard, D. Cobden and P. Lindelof, Nature **408**, 342 (2000).
8. S. De Franceschi *et al.*, cond-mat/0203146.
9. P. W. Anderson, J. Phys. C **3**, 2436 (1966).
10. K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
11. N. Andrei, Phys. Rev. Lett. **45**, 379 (1980); N. Andrei, K. Furuya and J.H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983).
12. I. Affleck and A. W. W. Ludwig, Nucl. Phys. B **360**, 641 (1991).
13. J. Kroha and P. Wölfle, in press (Springer), cond-mat/0105491.
14. A. Rosch, J. Kroha and P. Wölfle, Phys. Rev. Lett. **87**, 156802 (2001).
15. J. Appelbaum, Phys. Rev. Lett, **17**, 91 (1966); Phys. Rev. **154**, 633 (1967).
16. J. König, J. Schmid, H. Schoeller, and G. Schön, Phys. Rev. B **54**, 16820 (1996).
17. A.Rosch, J. Paaske, J. Kroha and P. Wölfle, cond-mat/0202404.
18. L.I. Glazman, private communication.
19. A.A. Abrikosov, Physics **2**, 21 (1965).
20. O. Parcollet, and C. Hooley, cond-mat/0202425.
21. H. Schoeller and J. König, Phys. Rev. Lett. **84**, 3686 (2000); see also M. Keil, Ph.D. thesis, U. Göttingen (2002).
22. D.C. Ralph and R.A. Buhrman, Phys. Rev. Lett. **72**, 3401 (1994).