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The atomic approach for the Anderson impurity model under an applied magnetic field

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We study the effect of a magnetic field applied on a localized level, described by the single impurity Anderson Hamiltonian (SIAH). We find approximate Green's functions (GF) for this case using the atomic approach. The starting point of this approach is the exact solution of the Anderson impurity in the zero bandwidth limit, then knowing the eigenenergies and eigenstates we calculate approximate GF. To obtain reliable results we impose the satisfaction of a generalized Friedel sum rule, which takes into account the applied magnetic field on the impurity. With the approximate GF, we obtain the Kondo splitting, above some critical value, about 0, 3TK, where TK is the impurity Kondo temperature.

Keywords: Atomic approach;Anderson impurity;heavy fermions.

Estudiamos el efecto de un campo magnético aplicado sobre un nivel localizado, descrito por el Hamiltoniano de Anderson de una sola impureza (HASI). Encontramos funciones de Green (FG) aproximadas para este caso usando el método atómico. El punto de partida de este método es la solución exacta del HASI en el límite de la banda estrecha, luego conociendo las auto-energías y los auto-estados, calculamos la FG aproximada. Para obtener resultados confiables, imponemos que sea satisfecha una regla de suma generalizada de Friedel, que toma en cuenta el campo magnético aplicado sobre la impureza. Con la FG aproximada obtenemos una quiebra del pico de Kondo por encima de un valor crítico alrededor de 0, 3Tk.

Descriptores: Enfoque atomic;impureza de Anderson;fermiones pesados.

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1. Introduction

Quantum dots are systems where a confinement potential allows discrete energy levels which resemble real atoms, this is an advantage because in bulk systems its intrinsic parameters are uncontrollable, whereas QD's offer the possibility of a complete control over all the relevant parameters of the model.

The main objective of this paper is to show, with a method developed by some of us [2], an effect pointed out by Costi [3] and later measured by Kogan *et al*. [4]; the splitting of the Kondo peak when a magnetic field is applied just over the impurity. This splitting appears above a critical value where the system is no longer in the Kondo regime. The direct evidence of this effect was given by Kogan [5], who measured the differential conductance as a function of drain and source voltages for different values of an applied magnetic field B.

The theoretical approach that will be used here, called the "atomic method" [2] is an approximate solution useful to study nanoscopic systems that exhibit Kondo effect. This approach is based on an adequate choice for an effective cumulant in the Green function and is a good candidate to describe strongly correlated impurity systems like QD's, because of its simplicity, low computational cost and good agreement with other reliable methods, like NRG approach and the non-crossing approximation (NCA).

The In Sec. 2 we introduce the single impurity Anderson Hamiltonian (SIAH) in the limit of infinite correlation ($U \to \infty$) and we highlight the usefulness of Hubbard operators Xpq in this limit. In Sec. 3 we derive the atomic method through the exact solution of the Anderson impurity model in the limit of zero conduction bandwidth. In Sec. 4 we show the splitting of the Kondo peak and discuss its relation with a possible transition between a singlet and doublet as fundamental states. Finally in the Appendix we present the details of the calculation of the exact Green's function for finite magnetic field $\vec{B}$ in the limit of zero conduction bandwidth.

2. The Anderson impurity model

The single impurity Anderson Hamiltonian is given by:

$$H = \sum_{\sigma} E_{f,\sigma} c^{\dagger}_{f,\sigma} c_{f,\sigma} + U n_{f,\sigma} n_{f,\bar{\sigma}} + \sum_{k,\sigma} E_{k,\sigma} c^{\dagger}_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \left(V_{f,k} c^{\dagger}_{f,k} c_{k,\sigma} + V^{*}_{f,k} c^{\dagger}_{k,\sigma} c_{f,\sigma} \right), \quad (1)$$

Where the two first terms in the upper line give the energy levels for the impurity, and the third term gives the kinetic energy of electrons in the leads. In the second line appears the hybridization energy between the impurity and free electrons. The correlation energy U is positive defined and is responsible for the double occupancy state.

In the strong Coulomb repulsion limit $U \to \infty$, if we are interested just in the low energy theory, there are high-lying eigenstates of the hamiltonian H that we do not consider. Then, we can obtain an effective lowenergy theory forbidding the double occupancy state in the fermionic operators, $|\uparrow\downarrow\rangle$, for some representation of the algebra $(c_{f,\mu}, c^{\dagger}_{f,\upsilon}) = \delta^{\mu}_{\upsilon}$, $(c_{f,\mu}, c_{f,\upsilon}) = 0$. Although the last procedure seems to be trivial, it is not, because the new effective operators no longer satisfy anticonmutation rules. We write the new operators in the next way, $c_{f\sigma} \to X^{0,\sigma}_{f} c^{\dagger}_{f\sigma} \to X^{\sigma,0}_{f}$, they satisfy the product rule, $X^{pq}_{f} X^{rs}_{f} = \delta^{q}_{r} X^{ps}_{f}$, which is a feature of Hubbard operators [6]. Then, under the strong Coulomb repulsion we write the SIAH in terms of Hubbard operators and Fermi operators as,

$$H = \sum_{\sigma} E_{f,\sigma} X^{\sigma,\sigma}_{f} + \sum_{k,\sigma} E_{k,\sigma} c^{\dagger}_{k,\sigma} c_{k,\sigma} + \sum_{\sigma} \left(V_{f,k} X^{\sigma,0}_{f} c_{k,\sigma} + V^{*}_{f,k} c^{\dagger}_{k,\sigma} X^{0,\sigma}_{f} \right) \qquad (2)$$

Despite of the fact that the Hamiltonian is now linear in the Hubbard operators and bilinear in Fermi operators, the equation of motion for the Green's functions is not simple, because the conmutator or anticonmutator of Hubbard operators is not a c-number, then the diagrammatic methods based on Wick's theorem are not applicable.

Now, a magnetic field is applied along the z-direction just on the magnetic impurity. Due to the presence of the magnetic field we add a Zeeman term to the SIAH that is given by the product of the z-component of the impurity spin, the intensity of the field, the Landé factor and the Bohr magneton, $H_Z = (\mu B g/2\hbar) B (X^{\uparrow,\uparrow}_{f} - X^{\downarrow,\downarrow}_{f})$. The resultant effect is to split the impurity level into two levels with different energies, their difference is given by $(\mu B g/\hbar)\, B$.

3. The atomic approach

The atomic method was developed in an earlier work [2], and in this approach we obtain an explicit expression for the atomic cumulant $M^{at}_{2,\sigma}(Z)$ in terms of $G^{at}_{ff,\sigma}(Z)$, where this GF is calculated in the Appendix A

$$M^{\text{at}}_{2,\sigma}(Z) = \frac{G^{\text{at}}_{ff,\sigma}(Z)}{1 + G^{\text{at}}_{ff,\sigma}(Z) (V)^2 \Sigma_k G^{o}_{c,\sigma}(k,Z)} \qquad (3)$$

The contribution of the c electrons was overestimated by concentrating them at a single energy level, and to moderate this effect we shall replace V^2 by Δ^2, where $\Delta = \pi V^2/2D$ is of the order of the width of the Kondo peak. As $M^{at}_{2,\sigma}(Z)$ is k independent, we can easily obtain, for a square band of bandwidth 2D, the approximate local Green function of the Anderson impurity:

$$G^{\text{imp}}_{ff,\sigma}(Z) = \frac{M^{\text{at}}_{2,\sigma}(Z)}{1 + M^{\text{at}}_{2,\sigma}(Z) \frac{(V)^2}{2D} \ln\left(\frac{Z+D+\mu}{Z-D+\mu}\right)} \qquad (4)$$

In the same way we can calculate the conduction and mixed GF's [2]. The difference between the exact and the approximate GF's is that different energies $E_{k,\sigma}$ appear in the c-electron propagators of the effective cumulant $M^{\text{eff}}_{2,\sigma}(Z)$, while these energies are all equal to the atomic conduction level E_0 in $M^{\text{at}}_{2,\sigma}(Z)$. Although $M^{\text{at}}_{2,\sigma}(Z)$ is for that reason only an approximation, it contains all the diagrams that should be present, and one would expect that the corresponding GF would have fairly realistic features. One still has to decide what value of E_q should be taken. As the most important region of the conduction electrons is the chemical potential μ, we will make satisfy the approximate GF a generalized Friedel sum rule proposed by Costi. With the fulfillment of the Friedel sum rule by the approximate GF, we find the adequate value for Eq.

The Friedel's sum rule at zero B [7] gives at T = 0, a relationship between the extra states induced below the Fermi level by a scattering center and the phase shift at the chemical potential $\eta_{\sigma}(\mu)$, obtained by the transference matrix $T^{s}_{\sigma}(Z) = V^2 G^{\text{imp}}_{ff,\sigma}(Z)$, where V is the scattering potential. For the AIM the extra states induced are given by the occupation number $n_{f,\sigma}$ of the localized state, and the scattering potential is the hybridization that affects the conduction electrons. The Friedel's sum rule for the Anderson impurity model at finite B can be writen as [3]

$$\rho_{f,\sigma}(\mu) = \frac{\sin^2 \pi n_{f,\sigma} (1 + \sigma M)}{\Delta \pi} \qquad (5)$$

where $\rho_{f,\sigma}(\mu)$ is the density of states of the localized level at the chemical potential, $n_{f,\sigma}$ are the occupation numbers and M is the magnetization such as that in the Stoner model.

4. Results

In Fig. 1 we plot the densities of states of the localized level for spin $\uparrow$ and $\downarrow$, ρ_{σ}, as a function of the frequency ω for a magnetic field applied just on the impurity. The magnetic field B is given in units of energy, $(\mu_B g B/\hbar)$. The particular value is 0, 9Tk where Tk is the Kondo temperature, defined as the mean width of the Kondo peak at zero magnetic field. In this figure we can see for each spin degree of freedom two peaks; one is the resonant peak that is centered at -0, 07, and the other is closed to the chemical potential μ = 0. The shifting of the Kondo peak is the main effect of the applied magnetic field, without it the Kondo peak must appear at the chemical potential μ = 0. For finite B the Zeeman term splits degenerated levels like doublets, triplets, etc. and transitions and eigenenergies are different for the system at zero B. For instance, in the atomic approach Fig. 4, we see that the singlet state 9 is the lowest energy state, and the first excited state is the 11th that forms a doublet. Then, for strong magnetic fields, a competition for the fundamental state starts because of the Zeeman splitting and the Kondo peak will disappear when the singlet state is no longer the many body fundamental state.

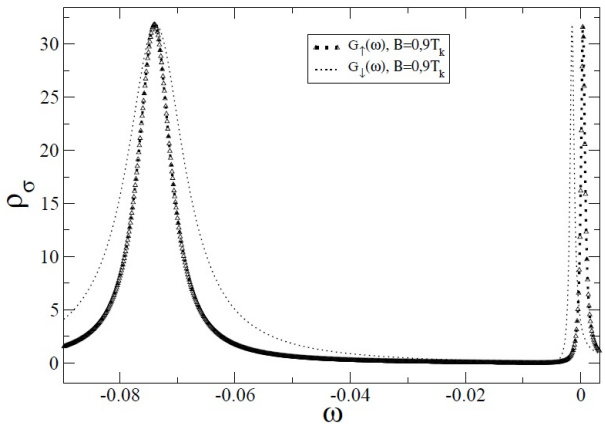

FIGURE 1. Density of states for each spin degree of freedom as a function of the frequency when a magnetic field is applied.

In Fig. 2 we plot the total density of states, $\rho\uparrow + \rho\downarrow$, for five finite values of B. We show just the region close to $\mu = 0$. For a low magnetic field 0, 1Tk, the kondo peak still exists, but for B = 0, 3Tk the height of the peak decreases and the former Kondo peak has split into two new peaks. For higher values of the magnetic field ˜B, the splitting continues and the two peaks structure is well formed. Our results are not identical to those of Costi [3] because the parameters are different, for example here the Kondo temperature is TK = 0, 00043 and in the article of Costi was 0, 0023, however the spirit is the same, we find that above a critical value (B = 0, 3Tk), the Kondo peak splits.

Another interesting effect that we have observed is that for large magnetic fields the spin down density of states broadens at the resonant band, Fig. 3. The effect in the spin up density of states is the opposite. Our interpretation of this effect is that more free electrons interact with the lower energy delocalized level due to the Zeeman effect. As the energies involved in this region are higher, this effect is not simple to see in the NRG approach, it would be interesting to test it with higher energy numerical approaches like density matrix renormalization group DMRG.

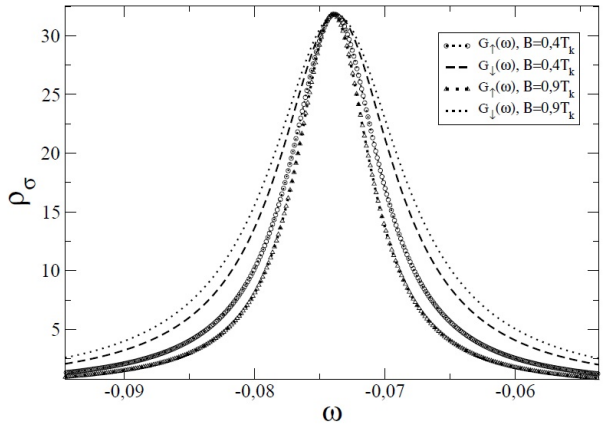

FIGURE 2. Total density of states $\rho\uparrow + \rho\downarrow$ close to the chemical potential, plotted for different values of B.

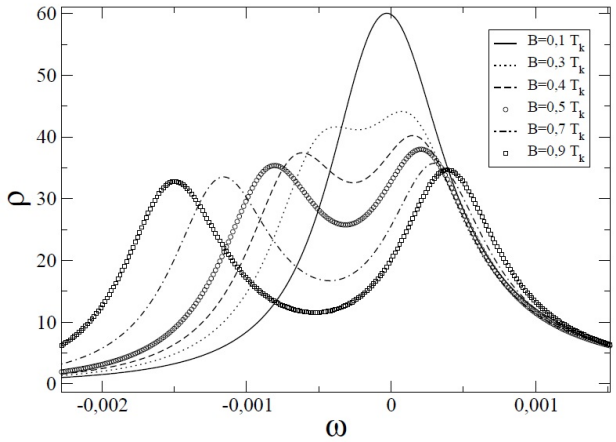

FIGURE 3. Resonant band for each spin degree of freedom. We can see that when a magnetic field is applied, the spin down density in this region broadens.

5. Conclusions

Based on the atomic approach for the SIAH, we were able to find an adequate cumulant for the impurity GF (3). This approximate cumulant was obtained by satisfying a generalized Friedel sum rule (5), that take into account of an applied magnetic field on the impurity. With the approximate GF we obtained the appearance of the Kondo splitting above some critical value, that we stated here about 0, 3Tk. We also noticed the broadening of the spin down density of states for finite B and we interpreted it saying that due to the Zeeman term in the SIAH, more free electrons interact with the localized spin down level than the spin up, via the hybridization.

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Appendix A: The Exact GF in the atomic limit

In the SIAH, the possible occupations of the conduction electrons at any site are four: (0, ↑, ↓, ↑↓), while at the impurity site the occupation of the local f electrons can be $(0, +1/2, -1/2)$, due to the restriction of the double occupation (U $\rightarrow \infty$). In the atomic case we have a Fock space with twelve states that we can diagonalize quickly finding the eigenenergies and eigenstates as can be seen in table (I).

In Fig. 4 we present the energy levels for our approximate hamiltonian, as well as their corresponding elementary excitations. The different transitions occur between states with n and n + 1 particles that satisfy $\langle n-1, j|X_{0\sigma}|n, j\rangle \neq 0$ and in the figure are represented by dash or dot lines if we are talking about $G^{at}_{\uparrow}(\omega)$ and $G^{at}_{\downarrow}(\omega)$, respectively. The levels depicted in this figure are obtained from table I, fourth column, in the presence of a magnetic field B = 0.9Tk and

TABLE I.Energies En,r of the atomic hamiltonian H. Columns indicate the number of electrons n, the name of the state r, the spin component Sz, the energies measured with respect the chemical potential, and the eigenstates |n, r ⟩. The factors xi, where x = a, b, c and i = 1, 2, 3 are responsible for the orthonormality in the subspace n = 2, they are given in terms of _i which are the roots of a third degree polynomial.

n	r	S_z	E_n, r	Eigenstates
0	1	0	0	$\|0,0\rangle$
1	2	$-\frac{1}{2}$	$\frac{\xi_q+E_f-\delta-\Delta'}{2}$	$\sin\alpha\|\downarrow,0\rangle - \cos\alpha\|0,-\frac{1}{2}\rangle$
1	3	$\frac{1}{2}$	$\frac{\xi_q+E_f+\delta-\Delta'}{2}$	$\sin\theta\|\uparrow,0\rangle - \cos\theta\|0,\frac{1}{2}\rangle$
1	4	$-\frac{1}{2}$	$\frac{\xi_q+E_f-\delta+\Delta'}{2}$	$\cos\alpha\|\downarrow,0\rangle + \sin\alpha\|0,-\frac{1}{2}\rangle$
1	5	$\frac{1}{2}$	$\frac{\xi_q+E_f+\delta+\Delta'}{2}$	$\cos\theta\|\uparrow,0\rangle + \sin\theta\|0,\frac{1}{2}\rangle$
2	6	-1	$E_f+\xi_q-\delta$	$\|\downarrow,-\frac{1}{2}\rangle$
2	7	0	λ_1	$a^1\|\uparrow\downarrow,0\rangle + b^1\|\downarrow,\frac{1}{2}\rangle + c^1\|\uparrow,-\frac{1}{2}\rangle$
2	8	1	$E_f+\xi_q+\delta$	$\|\uparrow,\frac{1}{2}\rangle$
2	9	0	λ_0	$a^0\|\uparrow\downarrow,0\rangle + b^0\|\downarrow,\frac{1}{2}\rangle + c^0\|\uparrow,-\frac{1}{2}\rangle$
2	10	0	λ_1	$a^2\|\uparrow\downarrow,0\rangle + b^2\|\downarrow,\frac{1}{2}\rangle + c^2\|\uparrow,-\frac{1}{2}\rangle$
3	11	$-\frac{1}{2}$	$E_f+2\xi_q-\delta$	$\|\uparrow\downarrow,-\frac{1}{2}\rangle$
3	12	$\frac{1}{2}$	$E_f+2\xi_q+\delta$	$\|\uparrow\downarrow,\frac{1}{2}\rangle$

with the fulfillment of the Friedel sum rule. The parameters employed in that table are, $\Delta = \sqrt{(\xi_q - E_{1/2})^2 + 4V^2}$, $\Delta' = \sqrt{(\xi_q - E_{-1/2})^2 + 4V^2}$, $\tan\alpha^+ 2V/(\Delta - E_{1/2} + \xi_q)$, and $\tan\alpha^+ 2V/(\Delta' + \xi_q - E_{-1/2})$.

To obtain the atomic Green's functions of the impurity in the zero bandwidth limit, we use the Zubarev's [9] equation

$$G^{at}_{\mu}(\omega) = e^{\beta\Omega}\sum_{n}\sum_{jj'}\left(e^{-\beta E_{nj}} + e^{-\beta E_{n-1j'}}\right) \times \frac{\left|\langle n-1, j', |X_\mu|, nj\rangle\right|^2}{\omega - (E_{nj} - E_{n-1j'})} \qquad \text{(A1)}$$

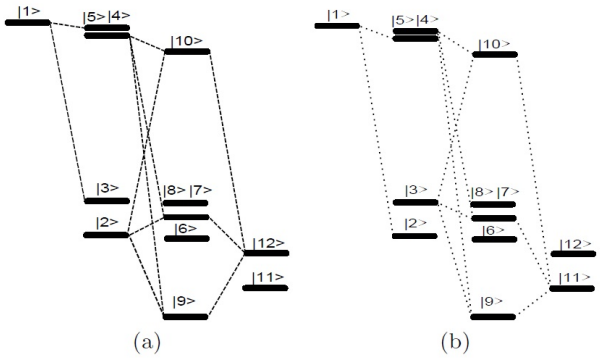

FIGURE 4. Energies of the 12 eigenstates of the zero conduction bandwidth limit of the Anderson model. The index r that characterizes the states is written above the corresponding levels. Dash lines (a) indicate the possible transitions involved in the up Green function, dot lines (b) are for the down Green function.

where Ω is the thermodynamical potential and the eigenvalues Enj and eigenvectors $((nj))$ correspond to the complete solution of the atomic Hamiltonian. The final result is the following

$$G^{at}(\omega) = e^{\beta\Omega}\frac{\sum_{i=1}^{11} m_i}{\omega - u_i} \qquad \text{(A2)}$$

where the poles and residues of the GFs $G^{\uparrow}_{at}(\omega)$ and $G^{\downarrow}_{at}(\omega)$ are given in terms of combination of factors in table I.

1. M. Vojta, R. Bulla, and W. Hofstetter, *Phys. Rev. B* **65** (2002) 140405.
2. T. Lobo, M. S. Figueira, and M.E. Foglio, *Nanotechnology* **17** (2006) 6016; *Nanotechnology* **21** (2010) 274007.
3. T.A. Costi, *Phys. Rev. Lett.* **85** (2000) 1504.
4. A. Kogan *et al.*, *Phys. Rev. Lett.* **93** (2004) 166602.
5. A. Kogan, G. Granger, M.A. Kastner, D. Goldhaber Gordon, and H. Shtrikman, *Phys. Rev. B* **67** (2003) 113309.
6. J. Hubbard, *Proc. R. Soc. London, Ser. A* **277** (1964) 237.
7. D.C. Langreth, *Phys. Rev.* **150** (1966) 516.
8. A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambrige Univ. Press, Cambridge, UK, 1993).
9. D.N. Zubarev, *Sov. Phys. Uspekhi* **3** (1960) 320.