NRG Study of an Inversion-Symmetric Interacting Model: Universal Aspects of its Quantum Conductance

Axel Freyn, Jean-Louis Pichard

NRG Study of an Inversion-Symmetric Interacting Model: Universal Aspects of its Quantum Conductance

Axel Freyn* and Jean-Louis Pichard
Service de Physique de l'État Condensé (CNRS URA 2464), IRAMIS/SPEC, CEA Saclay, 91191 Gif-sur-Yvette, France

We consider scattering of spinless fermions by an inversion-symmetric interacting model characterized by three parameters (interaction U, internal hopping t_d and coupling t_c). Mapping this spinless model onto an Anderson model with Zeeman field, we use the numerical renormalization group for studying the particle-hole symmetric case. We show that the zero temperature limit is characterized by a line of free-fermion fixed points and a scale $\tau(U, t_c)$ of t_d for which there is perfect transmission. The quantum conductance and the low energy excitations of the model are given by universal functions of t_d/τ if $t_d < \Gamma$ and of t_d/t_c^2 if $t_d > \Gamma$, $\Gamma = t_c^2$ being the level width of the scatterer. This universal regime becomes non-perturbative when U exceeds Γ.

PACS numbers: 71.10.-w,72.10.-d,73.23.-b

In quantum transport theory, the conductance G of a nanosystem inside which the electrons do not interact is given by $g = G/(e^2/h) = |t_{ns}|^2$ when the temperature $T \to 0$, $|t_{ns}|^2$ being the probability for an electron at the Fermi energy E_F to be transmitted through the nanosystem. This Landauer-Buttiker formula can be extended to an interacting nanosystem, if it behaves as a non-interacting nanosystem with renormalized parameters. We study such a renormalization using the numerical renormalization group (NRG) algorithm [1, 2] and an inversion-symmetric interacting model (ISIM) which describes the scattering of spin-polarized electrons (spinless fermions) by an interacting region characterized by an internal hopping term t_d, a coupling term t_c and an interaction strength U. This model was used [3, 4] for studying the effect of an external scatterer upon the effective transmission of an interacting region, assuming the Hartree-Fock (HF) approximation. We revisit ISIM with the NRG algorithm for investigating non-perturbative regimes where other methods (NRG or DMRG algorithms) than the HF approach become necessary.

Quantum impurity models [1], as the Anderson model which describes a level with Hubbard interaction U coupled to a 3d bath of free electrons, were introduced to study the resistance minimum observed in metals with magnetic impurities. The Kondo problem refers to the failure of perturbative techniques to describe this minimum. The solution of these models by the NRG algorithm, a non-perturbative technique [1, 2] introduced by Wilson, is at the origin of the discovery of universal behaviors which can emerge from many-body effects. The observation [5] of the Kondo effect in semiconductor quantum dots has opened a second era for quantum impurity models, now used for modeling mesoscopic objects (single [6] or double [7] quantum dot systems) inside which electrons interact, in contact with baths of free electrons (large conducting non interacting leads).

Though the Kondo effect is induced by magnetic moments, it is also at the origin of spinless models, such as the interacting resonant level model [8] (IRLM) which describes a resonant level ($V_d d^\dagger d$) coupled to two baths of spinless electrons via tunneling junctions and an interaction U between the level and the baths. IRLM, which is often used for studying nonequilibrium transport [8, 9], is related to the Kondo model, the charge states $n_d = 0, 1$ playing the role of spin states. Both ISIM and IRLM are inversion symmetric and can exhibit orbital Kondo effects. However, the Zeeman field acting on the impurity is played by the hopping term t_d for ISIM, and by the site energy V_d for IRLM. Therefore, ISIM does not transmit the electrons without field, while IRLM does. The two-particle states have been given for ISIM [10].

For the particle-hole symmetric case [2], the Anderson model maps onto the Kondo Hamiltonian if $U > \pi\Gamma$, Γ being the impurity-level width. In that case, there is a non-perturbative regime where the temperature dependence of physical observables such as the impurity susceptibility is given by universal functions of T/T_K, T_K being the Kondo temperature. If $U < \pi\Gamma$, the impurity susceptibility can be obtained by perturbation theory. Mapping ISIM onto an Anderson model with a Zeeman field t_d, and assuming that the role of t_d should qualitatively resemble that of a finite temperature, we expect the following scenario for the ISIM conductance g of the particle-hole symmetric case: If $U > \pi\Gamma \propto t_c^2$, we expect a non-perturbative regime where g should be given by a universal function of t_d/τ independently of the values of U and t_c, with a scale $\tau(t_c, U)$ of t_d playing the role of a Kondo temperature T_K. If $U < \pi\Gamma$, the HF theory should correctly give g. This scenario will be more or less confirmed by extensive NRG calculations.

ISIM Hamiltonian: $H = H_{ns} + H_l + H_c$. The Hamiltonian of the interacting region (the nanosystem) reads:

$$H_{ns} = -t_d \left(c_0^\dagger c_1 + c_1^\dagger c_0\right) + V_G\left(n_0 + n_1\right) + U n_0 n_1 \,. \quad (1)$$

$c_x^\dagger$ and c_x are spinless fermion operators at site x and $n_x = c_x^\dagger c_x$. The leads are described by an Hamiltonian

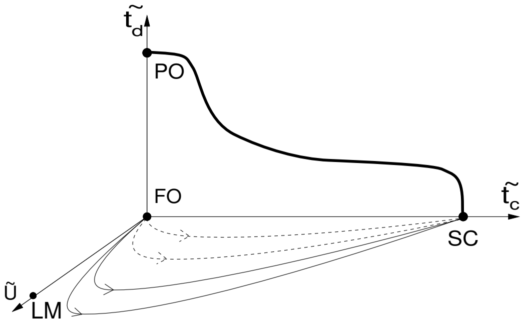

FIG. 1: Line of free fermion fixed points ($\tilde{U}=0$, thick solid line) characterizing ISIM when $T \to 0$ as t_d increases from $t_d = 0$ (SC fixed point) towards $t_d \to \infty$ (PO fixed point). The FO, LM and SC fixed points and the RG trajectories [1] followed by ISIM as T decreases for $t_d = 0$ are indicated in the plane $\tilde{t_d} = 0$, for $\pi\Gamma > U$ (dashed) and $\pi\Gamma < U$ (solid).

$H_l = -t_h \sum'^{\infty}_{x=-\infty} (c^\dagger_x c_{x+1} + H.c.)$, where $\sum'$ means that $x = -1, 0, 1$ are omitted from the summation. The coupling Hamiltonian $H_c = -t_c(c^\dagger_{-1} c_0 + c^\dagger_1 c_2 + H.c.)$.

Mapping onto an Anderson model with Zeeman field: Because of inversion symmetry, one can map ISIM onto a semi-infinite 1d lattice where the fermions have a pseudo-spin and the double site nanosystem becomes a single site with Hubbard repulsion U at the end point of the semi-infinite lattice. $a^\dagger_{\mathrm{e/o},x} = (c^\dagger_{-x+1} \pm c^\dagger_x)/\sqrt{2}$ creating a spinless fermion in an even/odd (e/o) combination of the orbitals at the sites x and $-x+1$ of the infinite lattice, (or a fermion with pseudo-spin $\sigma = $ e/o in a semi-infinite lattice), one gets $H_{ns} = (V_G - t_d)n_\mathrm{e} + (V_G + t_d)n_\mathrm{o} + U n_\mathrm{e} n_\mathrm{o}$, where $n_\sigma = a^\dagger_{\sigma,1} a_{\sigma,1}$ and where the pseudo-spin "e" ("o") is parallel (anti-parallel) to the "Zeeman field" t_d. In terms of the operators $d^\dagger_{k,\sigma} = \sqrt{2/\pi}\sum_{x=2}^{\infty} \sin(k(x-1)) a^\dagger_{\sigma,x}$ creating a spinless fermion of pseudo-spin σ and momentum k in the semi-infinite lattice, $H_l = \sum_{k,\sigma} \epsilon_k n_{k,\sigma}$ and $H_c = \sum_{k,\sigma} V(k)(a^\dagger_{\sigma,1} d_{k,\sigma} + H.c.)$, where the k-dependent hybridization $V(k) = -t_c\sqrt{2/\pi}\sin k$ yields an impurity level width $\Gamma = t_c^2$, $n_{k,\sigma} = d^\dagger_{k,\sigma} d_{k,\sigma}$ and $\epsilon_k = -2t_h \cos k$. ISIM is almost the Anderson model, except that the impurity has a Zeeman field t_d and is coupled to a semi-infinite 1d bath of free electrons. When $t_d \to 0$, ISIM exhibits an orbital Kondo effect if the equivalent Anderson model can be reduced to a Kondo model.

NRG procedure: ISIM can be studied using Wilson's procedure [1, 2] developed for the Anderson model after minor changes. First, we assume $V(k) \approx V(k_F = \pi/2)$ and, taking $\Lambda = 2$, we divide the conduction band (logarithmic discretization) of the electron bath into sub-bands characterized by an index n and an energy width $d_n = \Lambda^{-n}(1 - \Lambda^{-1})$. Within each sub-band, we introduce a complete set of orthonormal functions $\psi_{np}(\epsilon)$, and expand the lead operators in this basis. Dropping the terms with $p \neq 0$ and using a Gram-Schmidt procedure, the original 1d leads give rise to another semi-infinite chain with nearest neighbor hopping terms, each site being labelled by the same index n as the energy sub-band from which it comes, and representing a conduction electron excitation at a length scale $\Lambda^{n/2} k_F^{-1}$ centered on the impurity. In this transformed 1d model, the successive sites are coupled by hopping terms $t_{n,n+1} \propto \Lambda^{-n/2}$ which vanish as $n \to \infty$. The impurity and the $N-1$ first sites form a NRG chain of length N and of Hamiltonian H_N. This length can be interpreted [2] as a logarithmic temperature scale. The NRG chain coupled to the impurity is iteratively diagonalized and rescaled, the spectrum being truncated to the N_s first states at each iteration. The behavior of ISIM as T decreases can be obtained from the spectrum of H_N as N increases, the bandwidth of H_N being suitably rescaled at each step. A fixed point of the RG flow corresponds to an interval of successive even (or odd) values of N where the rescaled many-body excitations $E_I(N)$ do not vary. If it is a free-fermion fixed point, $E_I = \sum_\alpha \epsilon_\alpha$, the ϵ_α being one-body excitations, and the interacting system behaves as a non-interacting system ($\tilde{U} = 0$) with renormalized parameters $\tilde{t_d}$ and $\tilde{t_c}$ near the fixed point. Moreover, if one has free fermions when $T \to 0$, g can be extracted from the NRG spectrum.

Symmetric case: Using this NRG procedure, ISIM can be studied as a function of T for arbitrary values of its bare parameters. Hereafter, we take $t_h = 1$, $E_F = 0$ and $V_G = -U/2$. This choice makes ISIM invariant under particle-hole symmetry, with a uniform density ($\langle n_x \rangle = 1/2$) and 3 effective parameters ($\tilde{U}, \tilde{t_c}, \tilde{t_d}$).

Suppression of the LM fixed point as t_d increases: When $t_d = 0$, ISIM is an Anderson model which has the RG flow sketched in Fig. 1 for the particle-hole symmetric case. At low values of N (high values of T), ISIM is located in the vicinity of the unstable free orbital (FO) fixed point. As N increases (T decreases), ISIM flows towards the stable strong coupling (SC) fixed point. If $\pi t_c^2 < U$, the flow can visit an intermediate unstable fixed point: the local moment (LM) fixed point before reaching the SC fixed point. In that case, ISIM is identical to a Kondo model characterized by a temperature T_K and by universal functions of the ratio T/T_K. If $\pi t_c^2 > U$, the flow goes directly from the FO fixed point towards the SC fixed point, and there is no orbital Kondo effect for $t_d \to 0$. In Fig. 2(a), the first many-body excitations E_I of ISIM are given for increasing even values of N for $t_d = 0$. Since $\pi t_c^2 < U$, one gets 3 plateaus corresponding to the 3 expected fixed points. Inside the plateaus, the spectra are free-fermions spectra which are described in Ref. [2]. However, between the plateaus, there are no free-fermion spectra and $E_I \neq \sum_\alpha \epsilon_\alpha$. As t_d increases (Fig. 2(a)), the LM plateau decreases and vanishes when $t_d \approx U$.

Evolution of the SC fixed point as t_d increases: In the limit $N \to \infty$ ($T \to 0$), let us study the E_I as a

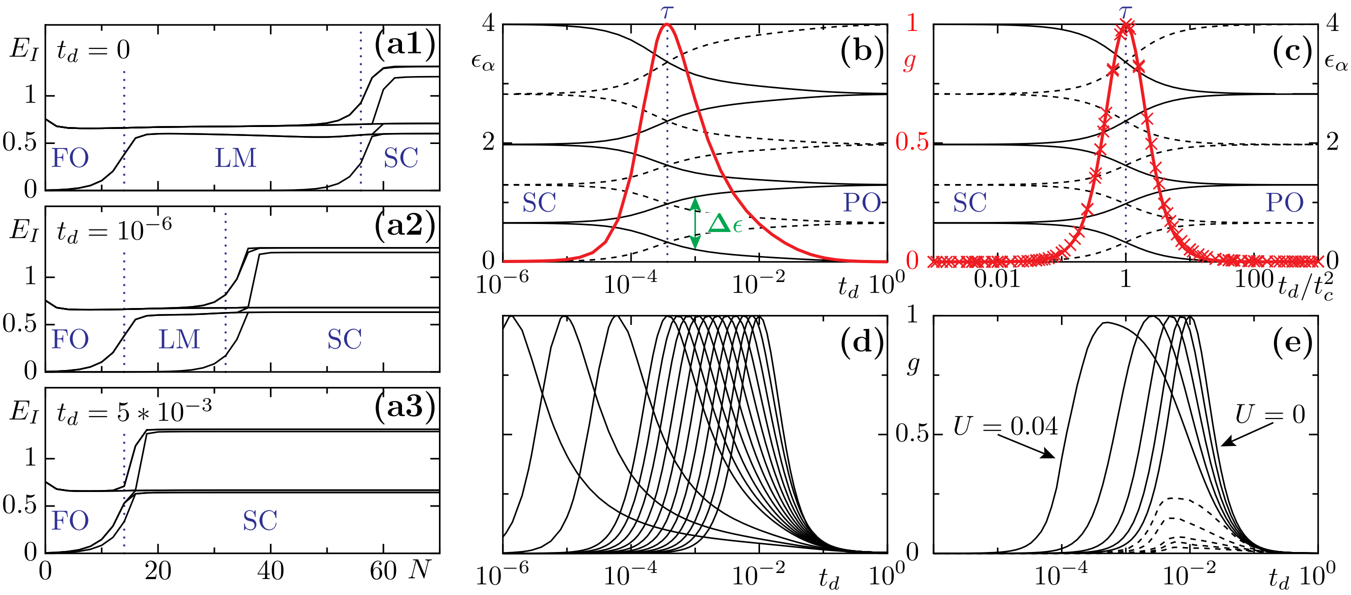

FIG. 2: (Color online) Fig. 2(a): Many body excitations E_I as a function of N (even values) for $U = 0.005$ and $t_c = 0.01$. For $t_d = 0$ (Fig. 2(a1)), one can see the 3 successive plateaus (FO, LM and SC fixed points) of the Anderson model [2]. As t_d increases (Fig. 2(a2) and Fig. 2(a3)), the LM plateau shrinks and disappears when $t_d \approx U$. Fig. 2(b): One body excitations $\epsilon_\alpha(t_d)$ (extracted from the $E_I(N \to \infty, t_d)$) for $U = 0.1$ and $t_c = 0.1$ (left scale). The solid (dashed) line corresponds to NRG chains of even (odd) length N. Conductance $g(t_d)$ extracted from $\Delta\epsilon(t_d)$ using Eq. (2) (thick red curve, right scale). For $t_d = \tau$, the ϵ_α are independent of the parity of N and $g = 1$. Fig. 2(c): For $U = 0$, $\epsilon_\alpha(t_d/t_c^2)$ and $g(t_d/t_c^2)$ extracted from the NRG spectra ($\times$). $g = \cosh^{-2}(X)$ (red line) with $X = \ln(t_d/t_c^2)$ is correctly reproduced. Figs. 2(d),(e): $g(t_d)$ for $t_c = 0.1$ and many values of U, calculated by NRG algorithm (d) and by HF theory (e). In Fig. 2(d), the larger is U, the smaller is $t_d = \tau$ where $g = 1$. The curves correspond respectively to $U = 0.25, 0.2, 0.15$ (3 left peaks) and $U = 0.1, 0.09, \ldots, 0.01, 0$ (11 right peaks). In Fig. 2(e), the HF values are accurate for $U = 0.02, 0.01, 0$ (3 right peaks), but become inaccurate when $U \approx 0.04 \approx \Gamma$. For $U > \Gamma$, the HF curves (dashed lines) are very different of the corresponding NRG curves (Fig. 2(d)).

function of t_d. For $t_d = 0$, one has the SC limit [2] where the impurity is strongly coupled to the second site (the conduction-electron state at the impurity site) of the NRG chain. The impurity and this site form a system which can be reduced to its ground state (a singlet), the $N-2$ other sites carrying free fermions excitations ϵ_α which are independent of that system. In the presence of a Zeeman field $t_d \neq 0$, the free-fermion rule $E_I(t_d) = \sum_\alpha \epsilon_\alpha(t_d)$ remains valid (see Fig. 2(b)) and the $T \to 0$ limit of ISIM is given by a continuum line of free-fermion fixed points where $\tilde{U} = 0$, as sketched in Fig. 1. When the pseudo-spin degeneracy is broken, the first (second) one-body excitation ϵ_1 (ϵ_2) carry respectively an even (odd) pseudo-spin if N is even. This is the inverse if N is odd, ϵ_1 (ϵ_2) carrying respectively an odd (even) pseudo-spin. For $t_d \to \infty$, the impurity occupation numbers $n_e = 1$ and $n_o = 0$, and the $N-1$ other sites of the NRG chain are independent of the impurity. We call this fixed point "Polarized Orbital" (PO), since it coincides with the FO fixed point of the Anderson model, except that the spin of the free orbital is fully polarized in our case. Since for $N \to \infty$ and $t_d \to 0$ (SC fixed point), the free part of the NRG chain has $N-2$ sites, while it has $N-1$ sites for $t_d \to \infty$ (PO fixed point), there is a permutation of the $\epsilon_\alpha(t_d)$ as t_d increases: as shown in Figs. 2(b) and (c), the $\epsilon_\alpha(t_d \to 0)$ for N even become the $\epsilon_\alpha(t_d \to \infty)$ for N odd and vice-versa.

Characteristic energy scale τ: We define the characteristic energy scale $\tau(t_c, U)$ of ISIM as the value of t_d for which the $\epsilon_\alpha(t_d)$ are independent of the parity of N when $N \to \infty$. Because of particle-hole symmetry, the nanosystem (the impurity of the NRG chain) is always occupied by one electron. Binding one electron of the leads with this electron reduces the energy when $t_d < \tau$, while it increases the energy when $t_d > \tau$. For $t_d = \tau$, it is indifferent to bind or not an electron of the lead with the one of the nanosystem, making ISIM perfectly transparent. This gives the proof that, for every values of U and t_c, there is always a value τ of t_d for which $g = 1$. The argument is reminiscent to that giving the condition for having a perfectly transparent quantum dot in the Coulomb blockade regime: t_d in our case, the gate voltage in the other case, have to be adjusted to values for which it costs the same energy to put an extra electron outside or inside the dot.

Extraction of the conductance g from the NRG spectra: If δ_e (δ_o) are the even (odd) scattering phase shifts at E_F,

$$g(t_d) = \sin^2(\delta_e - \delta_o) = \sin^2\left(\pi \frac{\Delta\epsilon(t_d)}{\Delta\epsilon(t_d \to \infty)}\right), \quad (2)$$

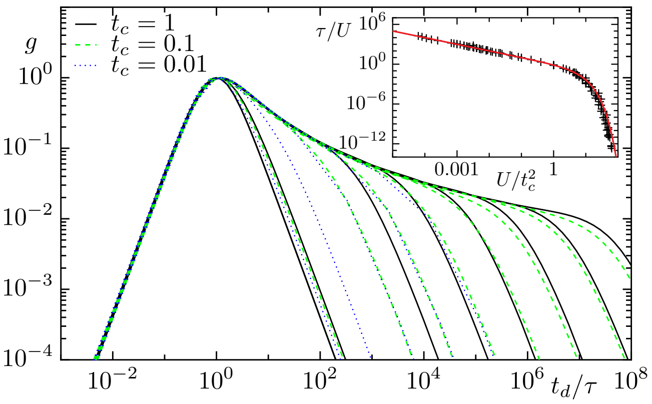

FIG. 3: (Color online) Conductance g as a function of t_d/τ for 3 values of t_c and many values $0 \leq U \leq 35$. Inset: $\tau(U, t_c)/U$ as a function of U/t_c^2 (+) and fit $\tau = t_c^2 \exp -(U/(\pi t_c^2))$ (solid red line).

where $\Delta\epsilon = \epsilon_2 - \epsilon_1$ is the energy gap between the two first excitations of a NRG chain of even length $N \to \infty$ (see Fig. 2(b)). When $U = 0$, this relation is a consequence of Friedel sum rule, which can be written for each pseudo-spin channel separately. In that case, $g = \cosh^{-2}(X)$ where $X = \ln(t_d/t_c^2)$ and $\tau = t_c^2$. The $\epsilon_\alpha(t_d)$ given by the NRG algorithm for $U = 0$ are shown in Fig. 2(c) with the corresponding values of g obtained from Eq. (2), showing that this procedure gives correctly g when $U = 0$. It has been shown [7, 11, 12] that Eq. (2) can also be used when $U \neq 0$, if there are free fermions when $T \to 0$.

Non-perturbative regime ($U > \Gamma/A$): In HF theory, t_d takes [3] a value $v = t_d + U\langle c_0^\dagger c_1(v, t_c)\rangle$ and $g = 1$ if $v = t_c^2$. This gives for the scale τ a HF value $\tau_{HF} = t_c^2 - AU$ where $A = \langle c_0^\dagger c_1(v = t_c^2, t_c)\rangle$ depends weakly on t_c, $A = 1/\pi$ (1/4) for $t_c = 1$ (0). When $U \to t_c^2/A$, $\tau_{HF} \to 0$, showing that HF theory cannot be used above an interaction threshold which is almost the threshold $\pi\Gamma$ giving the onset of the non-perturbative regime for the Anderson model. This breakdown of HF theory for $U \approx \Gamma/A$ can be seen if one compares Fig. 2(d) (NRG results) and Fig. 2(e) (HF results).

Universality: The conductance g extracted from the NRG spectra for $t_c = 0.01, 0.1$ and 1 and $0 \leq U \leq 35$ is given as a function of t_d/τ in Fig. 3. One can see 3 successive regimes. When $t_d < \tau$, there is a single curve which is independent of U and t_c and which corresponds to $g = \cosh^{-2}(X)$ with $X = \ln(t_d/\tau)$, and not $\ln(t_d/t_c^2)$ as for $U = 0$. When $t_d > \tau$, another universal curve independent of t_c and U describes the data as a function of t_d/τ as far as t_d does not exceed Γ. Indeed, the same data plotted as a function of t_d show that g becomes independent of U when $t_d > \Gamma$. In this third regime (parallel lines which can be seen in Fig. 3 for large values of t_d/τ) $g = \cosh^{-2}(X)$ with $X = \ln(t_d/t_c^2)$ as if $U = 0$.

Roles of T and t_d: We have assumed analogies between the effect of T in the Anderson model, the effect of a Zeeman field at $T = 0$ in the Anderson model, and eventually the effect of t_d at $T = 0$ in ISIM. This was based on the idea that the singlet state of the SC limit could be broken either if the temperature T or the Zeeman energy t_d exceeds T_K. Let us summarize the interest and the limit of these analogies. Increasing T in the Anderson model (or in ISIM with $t_d = 0$), one gets 3 regimes, each of them being characterized by a single fixed point (Fig. 2(a)). There are no free fermions for temperatures $T \approx T_K$ (SC–LM crossover) and $T \approx \Gamma$ (LM–FO crossover). In contrast, increasing t_d in ISIM at $T = 0$, one has always free fermions (Fig. 2(b)), and not only around 3 fixed points. However, there are 3 regimes in ISIM as t_d increases, as in the Anderson model as T increases, delimited by 2 energy scales τ and Γ. The behavior of $\tau \approx t_c^2 \exp -(U/(\pi t_c^2))$ (inset of Fig. 3) resembles that of $T_K \approx t_c\sqrt{\pi U/2} \exp -(U/(\pi t_c^2))$ (in ISIM units), while the second scale is given by Γ in the 2 models. Eventually, we point out the similarity between the universality discussed in this letter for g and that which characterizes [13] also at $T = 0$ the behavior of the singlet-triplet gap for a magnetic impurity confined in a box of mean level spacing Δ, as a function T_K/Δ.

We thank Denis Ullmo for very useful discussions and the "Triangle de la Physique" for financial support.

---

* Present address: Institut Néel, 25 avenue des Martyrs, BP 166, 38042 Grenoble, France.

[1] A. C. Hewson, *The Kondo Problem To Heavy Fermions* (Cambridge University Press, 1993).

[2] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980).

[3] Y. Asada, A. Freyn, and J.-L. Pichard, Eur. Phys. J. B **53**, 109 (2006).

[4] A. Freyn and J.-L. Pichard, Phys. Rev. Lett. **98**, 186401 (2007); A. Freyn and J.-L. Pichard, Eur. Phys. J. B **58**, 279 (2007); A. Freyn, I. Kleftogiannis, and J.-L. Pichard, Phys. Rev. Lett. **100**, 226802 (2008).

[5] D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav, and M. A. Kastner, Nature (London) **391**, 156 (1998).

[6] P. G. Silvestrov and Y. Imry, Phys. Rev. B **75**, 115335 (2007).

[7] L. Borda, G. Zaránd, W. Hofstetter, B. I. Halperin, and J. von Delft, Phys. Rev. Lett. **90**, 026602 (2003).

[8] P. Mehta and N. Andrei, Phys. Rev. Lett. **96**, 216802 (2006).

[9] E. Boulat, H. Saleur, and P. Schmitteckert, Phys. Rev. Lett. **101**, 140601 (2008).

[10] A. Dhar, D. Sen, and D. Roy, Phys. Rev. Lett. **101**, 066805 (2008).

[11] W. Hofstetter and G. Zarand, Phys. Rev. B **69**, 235301 (2004).

[12] A. Oguri and A. C. Hewson, J. Phys. Soc. Jpn. **74**, 988 (2005).

[13] R. K. Kaul, G. Zaránd, S. Chandrasekharan, D. Ullmo, and H. U. Baranger, Phys. Rev. Lett. **96**, 176802 (2006).