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

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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  $t_d/\tau$  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  $\Gamma$ .

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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  $U > \pi \Gamma$ ,  $\Gamma$ 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  $t_d/\tau$  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:

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

 $c_x^{\dagger}$  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).

 $\begin{array}{ll} H_l \ = \ -t_h {\sum'}_{x=-\infty}^{\prime \infty} (c_x^{\dagger} c_{x+1} + H.c.), \ \text{where} \ {\sum'} \ \text{means} \\ \text{that} \ x \ = \ -1, \ 0, \ 1 \ \text{are omitted from the summation.} \ \text{The} \\ \text{coupling Hamiltonian} \ H_c \ = \ -t_c (c_{-1}^{\dagger} c_0 + c_1^{\dagger} c_2 + H.c.). \end{array}$ 

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.  $a_{e/o,x}^{\dagger} = (c_{-x+1}^{\dagger} \pm c_{x}^{\dagger})/\sqrt{2}$ creating a spinless fermion in an even/odd (e/o) combination of the orbitals at the sites x and -x + 1of the infinite lattice, (or a fermion with pseudo-spin  $\sigma$  = e/o in a semi-infinite lattice), one gets  $H_{ns}$  =  $(V_G - t_d)n_e + (V_G + t_d)n_o + Un_e n_o$ , where  $n_\sigma = a_{\sigma,1}^{\dagger} a_{\sigma,1}$ and where the pseudo-spin "e" ("o") is parallel (antiparallel) to the "Zeeman field"  $t_d$ . In terms of the operators  $d_{k,\sigma}^{\dagger} = \sqrt{2/\pi} \sum_{x=2}^{\infty} \sin(k(x-1)) a_{\sigma,x}^{\dagger}$  creating a spinless fermion of pseudo-spin  $\sigma$  and momentum k in the semi-infinite lattice,  $H_l = \sum_{k,\sigma} \epsilon_k n_{k,\sigma}$  and  $H_c = \sum_{k,\sigma} V(k) (a_{\sigma,1}^{\dagger} d_{k,\sigma} + H.c.)$ , where the k-dependent hybridization  $V(k) = -t_c \sqrt{2/\pi} \sin k$  yields an impurity level width  $\Gamma = t_c^2$ ,  $n_{k,\sigma} = d_{k,\sigma}^{\dagger} d_{k,\sigma}$  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 semiinfinite 1d bath of free electrons. When  $t_d \rightarrow 0$ , 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 subbands 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  $\epsilon_{\alpha}$  being one-body excitations, and the interacting system behaves as a non-interacting system (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  $t_d \rightarrow 0$ . 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  $\epsilon_{\alpha}$  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  $\epsilon_{\alpha}$  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 U = 0, as sketched in Fig. 1. When the pseudo-spin degeneracy is broken, the first (second) one-body excitation  $\epsilon_1$  ( $\epsilon_2$ ) carry respectively an even (odd) pseudo-spin if N is even. This is the inverse if N is odd,  $\epsilon_1$  ( $\epsilon_2$ ) carrying respectively an odd (even) pseudo-spin. For  $t_d \to \infty$ , the impurity occupation numbers  $n_{\rm e} = 1$  and  $n_{\rm o} = 0$ , 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  $\tau$ : 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 Uand  $t_c$ , there is always a value  $\tau$  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  $\delta_e$  ( $\delta_o$ ) 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  $t_d/\tau$  for 3 values of  $t_c$  and many values  $0 \le U \le 35$ . 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 pseudospin 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  $\tau$  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  $U \rightarrow t_c^2/A$ ,  $\tau_{HF} \rightarrow 0$ , 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  $0 \le U \le 35$  is given as a function of  $t_d/\tau$  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  $t_d/\tau$  as far as  $t_d$  does not exceed  $\Gamma$ . 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  $t_d/\tau$ )  $g = \cosh^{-2}(X)$  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  $\tau$  and  $\Gamma$ . 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  $\Gamma$  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  $\Delta$ , as a function  $T_K/\Delta$ .

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