Local Kondo temperatures in atomic chains

R. R. Agundez,1 J. Salfi,2 S. Rogge,1,2 and M. Blaaugeo1

1Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands
2Centre for Quantum Computation and Communication Technology, University of New South Wales, Sydney NSW 2052, Australia

We study the effect of disorder in strongly interacting small dopant chains. Using the Kotliar-Ruckenstein slave-boson approach we diagonalize the Hamiltonian via scattering matrix theory. We numerically solve the Kondo transmission and the slave-boson parameters that allow us to calculate the Kondo temperature. We demonstrate that in the weak disorder regime, disorder in the energy levels of the dopants induces a non-screened disorder in the coupling energy between dopants. We find that this disorder in the couplings comes from a local distribution of Kondo temperatures along the chain. We propose an experimental setup where these local Kondo temperatures can be observed.

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One of the most studied phenomena in condensed-matter physics is electron localization in disordered systems. In one-dimensional systems, disorder and interactions play an important role in transport. In the limiting case of no electron-electron interactions ($U = 0$), we encounter Anderson localization for even the smallest disorder $1, 2$. When interactions dominate, the system is in a Mott insulator state $2, 3$. Both limiting cases have been extensively studied but much less is known in the intermediate regime. Even though disorder or electron interactions drive the system to an insulating phase, it has been proposed that in an intermediate regime a metallic phase should appear $4$. Electron-electron interactions can increase the conductance of a system in a disordered potential $5–8$. Interactions partially screen the disorder potential, and a fraction of the electrons undergo a Mott localization while the rest remain Anderson localized. The result is a gapless two-fluid phase called Mott-Anderson insulator $4$.

We propose chains of dopant atoms in silicon for the realization of interacting one-dimensional electronic systems. We envision few dopant systems fabricated with technology for placement of dopants with near-atomic precision by scanning tunneling microscopy (STM), or with few nm precision by ion implantation $9–12$. The single dopant undergoes a Mott localization while the rest remain Anderson localized. The result is a gapless two-fluid phase called Mott-Anderson insulator $4$.

We show that Coulomb interactions screen the disorder potential for weak disorder and therefore the Kondo transmission increases with increasing interactions. We demonstrate that the screened diagonal disorder induces a non-screened disorder in the coupling energy between dopants due to different local Kondo temperatures in the chain. Finally, we propose an experimental setup for the detection of such local Kondo temperatures.

Model. We consider a chain of $N$ dopant atoms connected to conducting leads. We model the structure as a chain of $N$ quantum dots (QDs) whose ends are attached to an electron bath with a dispersion energy given by $\epsilon_k = \epsilon_F - 2t_0 \cos k$. From now on we take $\epsilon_F = 0$. Fig. 1 shows a schematic representation of the system. We assume that each dopant has a single energy level labeled $\epsilon_i$ with $i = 1, 2, 3, ..., N$. The hopping energy between the chain and the left (right) lead is denoted by $t_L$ ($t_R$) and the hopping energy between QD $i$ and QD $i + 1$ is $t_i$. Finally, each of the dopants in the chain have an intra-Coulomb interaction $U$. The Hamiltonian of the system is given by

$$H = H_L + \sum_{i,\sigma} N \epsilon_i f_{i\sigma}^\dagger f_{i\sigma} - \sum_i (t_i f_{i+1\sigma}^\dagger f_{i\sigma} + c.c.)$$

$$- \sum_{\sigma} (t_L c_{-1}\sigma f_{1\sigma} + t_R c_{N}\sigma f_{N\sigma} + c.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

with $H_L = \epsilon_F \sum_{j\sigma} c_{j\sigma}^\dagger c_{j\sigma} - t_0 \sum_{j\sigma} (\epsilon_{j\sigma} c_{j+1\sigma} + c.c.)$ and $n_{i\sigma} = f_{i\sigma}^\dagger f_{i\sigma}$. The operators $c_{i,\sigma}(c_{i,\sigma}^\dagger)$ and $f_{i,\sigma}(f_{i,\sigma}^\dagger)$ correspond to the annihilation (creation) operators in the

![FIG. 1. Tight-binding model for a chain of QDs coupled to conducting leads.](image-url)
leads and in the QDs, respectively. Diagonal disorder ($W$) is introduced by randomly choosing $\epsilon_n$ from a uniform distribution centered around the electron-hole symmetry point $-\frac{U}{2}$, that is, $\epsilon_i = -\frac{U}{2} + \left[ \frac{W}{2}, \frac{W}{2} \right]$, such that for zero disorder the dopants are in the middle of the Coulomb blockade region. We apply the slave-boson approach of Kotliar and Ruckenstein (KR) \cite{12, 13} to treat the electron interaction $U$ in the system. This scheme introduces 4 boson creation (annihilation) operators $c_i^\dagger(\epsilon_i), p_{i\sigma}^\dagger(p_{i\sigma})$ and $d_i^\dagger(d_i)$ that act on each QD of the chain. Now the $c_i^\dagger |0\rangle_i, p_{i\sigma}^\dagger f_i^\dagger |0\rangle_i$, and $d_i^\dagger f_i^\dagger |0\rangle_i$ states represent the empty state, the singly occupied state and the doubly occupied state, respectively. $d_i^\dagger d_i$ thus represents the counting operator for the doubly occupied state. This change of basis is applied by replacing $f_i \rightarrow f_i z_i$. In the Hamiltonian $H$ [Eq. (1)], where $z_i = \sqrt{1-d_i^\dagger d_i-\lambda}$. Two constraints are applied to the bosons, namely the completeness relation: $\epsilon_i \epsilon_i + \sum \lambda_i^\dagger \lambda_i + d_i^\dagger d_i = 1$, and the correspondence condition between fermions and bosons: $p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i = f_i^\dagger f_i$. We add these two constraints to the Hamiltonian [Eq. (1)] by using the Lagrange multipliers $\lambda_i$ and $\gamma_i$. The new Hamiltonian is then $H_{SB} = H + \sum \lambda_i^\dagger \lambda_i + d_i^\dagger d_i - 1 + \sum \gamma_i p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i - f_i^\dagger f_i$. Following the steps of the KR method the four boson operators are replaced by their corresponding expectation values \cite{13, 14}. We then arrive at the following effective non-interacting Hamiltonian:

\begin{equation}
H_{\text{eff}} = H_L + \sum_{i=1}^{N} \epsilon_i f_i^\dagger f_i - \sum_{i=1}^{N-1} (t_iz_{i+1} f_i^\dagger f_{i+1} + c.c.) - (t_L z_i^\dagger f_1 + t_R z_{N-1}^\dagger f_N + c.c.).
\end{equation}

The energy levels in Eq. (2) have been renormalized to $\epsilon_i = \epsilon_i - \gamma_i$. We analytically diagonalize $H_{\text{eff}}$ [Eq. (2)] using scattering theory \cite{16}, and together with the KR equations:

\begin{align}
\frac{1}{2}(1 - \epsilon_i^2 + d_i^2) - \langle f_i^\dagger f_i \rangle &= 0 \quad (3a) \\
\frac{\partial_{\epsilon_i} R_i}{\partial \epsilon_i} R_i + \gamma_i \epsilon_i &= 0 \quad (3b) \\
d_i(U + \gamma_i) - \frac{\partial z_i}{\partial d_i} R_i &= 0. \quad (3c)
\end{align}

we solve the system self-consistently and obtain the Lagrange multipliers and bosonic expectation values. In Eq. (3) \( R_1 \equiv t_L ((c_i^\dagger f_1) + (f_i^\dagger c_{i-1})) + t_1 z_2 ((f_i^\dagger f_2) + (f_2^\dagger f_1)), \)

\( R_N \equiv t_{N-1} z_{N-1} ((f_{N-1}^\dagger f_N) + (f_N^\dagger f_{N-1})) + t_L ((f_1^\dagger c_N) + (c_1^\dagger f_N)) \) and \( R_i \equiv t_{i-1} z_{i-1} ((f_{i-1}^\dagger f_i) + (f_i^\dagger f_{i-1})) + t_i z_{i+1} ((f_i^\dagger f_{i+1}) + (f_{i+1}^\dagger f_i)). \)

We then use the parameters from Eq. (3) in the transmission expression derived via scattering theory. We also compute the value of the quasiparticle weight $z_n^2$ for each QD,

\begin{equation}
z_n^2 = \frac{2(\epsilon_i + d_i)^2[1 - (\epsilon_i^2 + d_i^2)]}{1 - (\epsilon_i^2 - d_i^2)^2}.
\end{equation}

This is a very important parameter in the description of the impurity problem. In the case of a single impurity, the Kondo temperature in our formalism is given by $T_{K, KR} = 2\Gamma$. If $U = 0$ the resonance level has the width $\Gamma = t_L + \Gamma_R$, we find $\gamma_i = 2t_i^2/t_0$, $l = L, R$. To demonstrate the validity of the approach, we show that the KR results for one quantum dot agree with the widely used expression for the Kondo temperature derived by Halvane [Fig. (4a)], \cite{17, 18}, and then perform calculations for more complicated systems.

**Results**.- Unless stated otherwise we work at zero temperature, take the wide band limit and the symmetric case: $t_1 = t_L = t_R = \frac{W}{2} = t$.

We show in Fig. 2 averaged values of conductance over 2000 random configurations for different disorder strengths. We observe that if $U$ increases conductance is less sensitive to disorder. We found that in the region $W < U$, the averaged quantum dot level values over the 2000 configurations $\epsilon_i$, had values closer to $\epsilon_F$, while for $W > U$ energy levels were not being pinned at the Fermi level anymore [Fig. (4a)]. This can be attributed to stronger Kondo screening of the disorder for larger values of $U$. For $W < U$ all energy levels lie inside the Coulomb blockade region, therefore all the QDs experience Kondo screening.

As the disorder $W$ increases to the region $W > U$, some of the energy levels can lie outside the Kondo regime (Coulomb blockade regime $-U < \epsilon_i < 0$). Therefore they will not be pinned to the Fermi level and there is no disorder screening. Since there is no screening by the Coulomb interaction in this region there is no dependence on $U$, so that all the curves merge for $W >> U$ regardless of $U$, as we observe in Fig. 2. For large enough disorder, on-site electron-electron interaction thus plays no role in the Kondo transmission.

In a plain Hubbard chain the dependence of the conductance on the energy scale $U/t$ can be identified quite easily by dividing the initial Hamiltonian by $t$ such that $U/t$ appears naturally as the energy scale. In this case the interplay of disorder $W$ and Coulomb interaction $U$ is more obscure, and the relevant scale is not naturally found as in the Hubbard case. Moreover the inset of Fig. 2 shows how the transmission lines lie on top of each other when disorder is re-normalized by $U$, pointing out that the transmission depends on disorder and Coulomb interaction only via the ratio $W/U$.

We have seen that in the region $W < U$, disorder is screened by interactions, therefore the energy levels of the dopants are pinned at the Fermi level due to the Kondo effect [Fig. (4a)]. Despite this fact we observe in Fig. 2 a monotonic decrease of transmission for $W < U$. We find that rather than the usual quenching of transmission by...
the direct diagonal disorder imposed in the Hamiltonian, here off-diagonal disorder indirectly appears. Diagonal disorder of the applied potential in Eq. (1) transforms into off-diagonal disorder of couplings in Eq. (2) via the $z_n$ terms. If disorder increases the values of each $z_n$ can lie in a broader distribution of quasiparticle values [Fig. 3 (b)-(d)], and it is the variation of $z_n$ among the sites which creates the monotonic decrease of transmission in the region $W < U$.

We know that the quasiparticle weight can range from 0, signaling the dominance of the Coulomb interaction, to 1, meaning that the spin is behaving freely. If the electrons feel a weak Coulomb interaction, the probability for any occupation number of the QD will be similar, so $e_i^2 = p_i^{2e} = d_i^2 \rightarrow \frac{1}{4}$, giving $z_i \rightarrow 1$. If there is a strong electron-electron interaction the energy level will try to be singly occupied, $p_i^2 = p_i^{2e} + p_i^{2\uparrow} \rightarrow 1$. Then $e_i^2$ and $d_i^2$ will tend to zero, giving $z_i^2 \rightarrow 0$. For small $W$ the distribution will lie in the lower part of the spectrum. As disorder increases to $W \approx U$ the $z_n$ can be seen to spread and when $W > U$ the distribution will again become narrower, but now around the upper part of the spectrum, signaling the dominance of disorder in the system.

We attribute this difference in Kondo temperatures of the impurities in a Kondo chain to the different screening strengths from the conduction electrons in the leads. For different positions in the chain the screening will be different. We have established that for a finite disorder, small enough to keep the dopants under Coulomb blockade, we have a different local Kondo temperature for each of the dopants. In principle this is enough for different Kondo temperatures to appear. In an experiment however $T_K$ is extracted by performing conductance measurements, which means that the temperature of the system needs to be at least on the order of $T_K$.

We begin by demonstrating the validity of our slave-boson approach. Fig. 4(a) shows that our results for one quantum dot agree with the widely used expression for the Kondo temperature derived by Haldane for a single Coulomb interacting quantum dot.

For our results presented in Fig. 4 we have used experimental parameters for donors in silicon. The on-site Coulomb repulsion has been estimated as $U \approx 50$ meV, the coupling between the elements of the chain is taken as $t_i = \frac{U}{10}$. This corresponds to a separation of the dopants in silicon of around 7 nm, which is a realistic experimental value.

We start by calculating the local $T_K$ for a chain of 3 QDs in a symmetric system with zero disorder [Fig. 3(b)]. This setup simulates an experiment performed in a symmetric arrangement of 3 quantum dots in series, attached to two conducting leads. Our calculations show that even though we get accessible Kondo temperatures for the system, these temperatures are roughly the same for each QD. Therefore in a symmetric non-disordered setup we do not expect a strong observation of different local Kondo temperatures along the chain.

Next we discuss an experimental setup where coupling to any localized state in the chain can be achieved using an STM operated at low temperature. We suppose the STM tip to be the right conducting lead with a coupling $\Gamma_R$ controlled by the tip height. To preserve Kondo physics, a left lead is defined as a highly doped reservoir with a coupling $\Gamma_L$ similar to the setup in Fig. 1. In a STM measurement the tunneling rate through vacuum to the tip, $\Gamma_R$, will be $\Gamma_R \ll \Gamma_L$ for the range of $\Gamma_L \geq 1$ meV needed for practical experiments on dopants with $U \sim 50$ meV. This will decrease $T_K$ in the QDs nearest to the right lead as they will experience less screening from the conduction electrons from that lead. In Figs.

![FIG. 2. Averaged conductance over 2000 random configurations versus disorder for a chain of $N = 3$ QDs for different strengths of electron-electron interaction. The inset shows the curves lying on top of each other when disorder is renormalized by $U$.](image2)

![FIG. 3. Calculations were performed using a chain of 3 QDs with a Coulomb interaction of $U = 10$. a) Renormalized energy level of the QDs in the chain averaged over 2000 configurations. b)-d) Distribution of the quasiparticle weight [Eq. 4] for $i = 1$ and $i = 2$ for all the different system configurations using different values of disorder such that $W < U$.](image3)
moving along the chain the weakest link can be identified, proving the existence of local Kondo temperatures in dopant chains.

Conclusion.- In this Letter we have shown the existence of induce disorder in the couplings between dopants in an atomic chain due to applied disorder in the energy levels, in the weakly disordered regime (W < U). Furthermore we predict different local Kondo temperatures in each of the dopants in the chain and suggested a STM experiment setup to observe the local Kondo temperature distribution in an atomic chain. This work is part of the research program of the Foundation for Fundamental Research on Matter (FOM), which is part of the Netherlands Organization for Scientific Research (NWO). This research was financially supported by the ARC Centre of Excellence for Quantum Computation and Communication Technology (CE110001027) and the Future Fellowship (FT100100589).

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