How sharply does the Anderson model depict a single-electron transistor?

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The single-impurity Anderson model has been the focus of theoretical studies of molecular junctions and the single-electron transistor, a nanostructured device comprising a quantum dot that bridges two otherwise decoupled metallic leads. The low-temperature transport properties of the model are controlled by the ground-state occupation of the quantum dot, a circumstance that recent density-functional approaches have explored. Here we show that the ground-state dot occupation also parametrizes a linear mapping between the thermal dependence of the zero-bias conductance and a universal function of the temperature scaled by the Kondo temperature. Careful measurements by Grobis and co-workers are very accurately fitted by the universal mapping. Nonetheless, the dot occupation and an asymmetry parameter extracted from the same mapping are relatively distant from the expected values. We conclude that mathematical results derived from the model Hamiltonian reproduce accurately the universal physical properties of the device. In contrast, non-universal features cannot be reproduced quantitatively. To circumvent this limitation, 

In this charged environment, the obstacle that lay ahead might have been disregarded, had Hardy and collaborators not issued the heads up. In an inspiring report, they showed that, unlike static DFT, the time-dependent formalism (TD-DFT) can climb the crossover 

This remarkable progress notwithstanding, some of the work that was done after Ref. \cite{16} came to light indicates that Hardy’s message has not come across clearly. Another shot seems in order.

The complexity of the crossover and its relation to high- and to the low-temperature properties can be perceived from another perspective, rooted in physical considerations. The crossover is due to the formation of the Kondo cloud. At high energies, if the gate voltage attracts an odd number of electrons, the dot acquires a magnetic moment. The dot moment is antiferromagnetically coupled to the moments of the nearby lead electrons. As the temperature $T$ is lowered past a characteristic temperature $T_K$ (the Kondo temperature, typically of the order of 1 K), a cloud arises in the leads that couples with the dot spin to form a singlet. Below $T_K$, the entanglement between the dot and lead electrons allows ballistic conduction across the device.

The cloud is large. The correlation length grows as the temperature is reduced, i.e., as the Hamiltonian crosses over from the high- to the low-temperature regimes, and may exceed $1 \mu$. Such long lengths introduce non-local effects that simple approximations to the static exchange-correlation functional are unlikely to capture. Discussion of the DFT approach from a strategic perspective seems

I. INTRODUCTION

Molecular junctions and analogous elementary nanostructured devices have motivated a great deal of experimental and theoretical research \cite{1–4}. Archetypical among such systems is the single-electron transistor (SET), a quantum dot or molecule (dot, for brevity) bridging two otherwise decoupled 2D electron gases or metallic leads (leads) \cite{5–8}. That the single-impurity Anderson Hamiltonian would model the transport properties of the device was realized well before the first SET was manufactured. Two corollaries emerged. First, in view of the universal properties of the Anderson Hamiltonian, quantitative interpretation of experimental data was envisaged. Second, given that the dot occupation controls the ground-state transport properties, the model invited Density-Functional Theory (DFT) treatment. With the invitation, alas, came a challenge.

A formidable barrier faces density-functional theorists interested in molecular junctions or SETs. A crossover separates the high-energy properties from the low-energy properties. The crossover is refractory to perturbative treatment. Only special methods can treat it.

At first, difficulties other than the crossover attracted attention \cite{9}. DFT is centrally concerned with the ground state; research was therefore focused on the low-temperature behavior, the transport properties being computed via Landauer-Büttiker formalism \cite{10}. With a view to developing trustworthy approximations for the exchange-correlation functional, accurate special results such as Density-Matrix Renormalization-Group data \cite{11}, the Friedel sum rule \cite{12}, the behavior of an isolated impurity in the low-temperature limit \cite{13}, and Bethe-Ansatz results for the ground-state occupancy of the Anderson-model impurity \cite{14,15} were invoked.
temperature. The linear coefficient is a trigonometric function of the ground-state phase-shifts induced by the screening of the dot moment. Here, we will allow for an external potential applied to the leads and take advantage of Friedel’s sum rule to relate the phase shifts to the $T \ll T_K$ and $T \gg T_K$ occupations of the dot orbital.

The schematic drawing in Fig. 1 defines the model. (For a micrograph of the modeled device, see Figure 1(a) in Ref. [21].) The quantum dot, at the center of the figure, is coupled to the left ($L$) and the right ($R$) leads with couplings $V_L$ and $V_R$, respectively. The dot-level energy, and hence the dot occupancy are controlled by the gate potential $V_G$. 

![Fig. 1](image_url)  

**FIG. 1:** (Color online) Single-electron transistor. The quantum dot is asymmetrically coupled to the left ($L$) and the right ($R$) leads, with couplings $V_L$ and $V_R$, respectively. The gate potential $V_G$ controls the dot energy. The arrows indicate the direction of conduction.

The Anderson Hamiltonian modeling the device in Fig. 1 reads

$$H_A = H_d + \sum_{k,\alpha=L,R} \varepsilon_k c_{k\alpha}^\dagger c_{k\alpha} + \frac{W}{N} \sum_{k,q,\alpha=L,R} c_{k\alpha}^\dagger c_{q\alpha}^\dagger + \frac{V_G}{\sqrt{N}} (c_d^\dagger c_{d\alpha} + H. c.).$$  

with implicit spin sums throughout. As usual, the dot Hamiltonian $H_d$ comprises a Coulomb repulsion $U$ and a dot energy $V_G$, defined by the gate potential. The two structureless conduction bands in the first term on the right-hand side represent the left- ($\alpha = L$) and the right-hand ($\alpha = R$) leads. The normalized sum $(1/\sqrt{N}) \sum_{k\alpha} \varepsilon_{k\alpha}$ defines the Wannier state in lead $\alpha$ to which the dot level $c_d$ is coupled.

The second term on the right-hand side of Eq. (1) represents equal external potentials applied to the same Wannier states. The potentials must be identical to maintain equilibrium, but the application to the orbitals coupled to the dot is by no means restrictive. Renormalization-group theory proves that substitution of a momentum-dependent form $\sum_{k,q,\alpha} W_{kq} c_{k\alpha}^\dagger c_{q\alpha}$ for the second term on the right-hand side would only add irrelevant terms to the Hamiltonian [22, 23].
Such irrelevant operators would contribute to physical properties at high energies. For decreasing temperatures, however, the contribution would decay in proportion to $T$, or more rapidly, and by no means affect the universal properties of the model. For practical purposes, therefore, Eq. (1) is sufficiently general.

### A. Decoupling of the model Hamiltonian

It is straightforward to construct linear combinations of the operators $c_{k\alpha}$ ($\alpha = L, R$) that are decoupled from the quantum dot [24]. To this end we define the orthonormal Fermi operators

\[
\begin{align*}
    a_k &= \frac{V_L c_{kL} + V_R c_{kR}}{V}, \\
    b_k &= \frac{V_R c_{kL} - V_L c_{kR}}{V},
\end{align*}
\]

where

\[ V \equiv \sqrt{V_L^2 + V_R^2}. \]

Projected on the basis of $a_k$’s and $b_k$’s, the Hamiltonian (1) reduces to the form

\[ H_A = H + \hat{H}, \]

where

\[ \hat{H} = \sum_k \epsilon_k b_k^\dagger b_k + \frac{W}{N} \sum_{k,q} b_k^\dagger b_q, \]

and

\[ H = H_d + \sum_k \epsilon_k a_k^\dagger a_k + W f_0^\dagger f_0 + V (c_d^\dagger f_0 + \text{H. c.}), \]

with the shorthand

\[ f_0 = \frac{1}{\sqrt{N}} \sum_k a_k. \]

The right-hand side of Eq. (7) is the standard expression for the single-impurity, single-band Anderson Hamiltonian [25]. The second band, defined by Eq. (6), is decoupled from the quantum dot and can be disregarded, for nearly all applications. Exceptions are the transport properties, to which the $b_k$’s contribute. To compute the zero-bias electrical conductance, for example, one must apply an infinitesimal bias

\[ H_\mu = \Delta \mu \sum_k \left( c_{kR}^\dagger c_R - c_{kL}^\dagger c_{kL} \right), \]

between the $L$ and the $R$ leads.

Projection of Eq. (9) upon the basis defined by Eqs. (2) shows that $H_\mu$ couples the $a_k$’s to the $b_k$’s. Likewise, the current operator $\hat{I} = \hat{q}_R/t$, where $\hat{q}_R$ is the electrical charge in lead $R$, couples the $a_k$’s to the $b_k$’s. Standard linear response theory links the conductance $G$ to the commutator between the bias $\hat{I}$ and the current $\hat{I}$.

This considered, one can follow the algebraic manipulations in appendix C of Ref. [20] to show that

\[ G(T) = \kappa \pi G_2 \Gamma_W \int \left( -\frac{\partial f}{\partial \epsilon} \right) \rho_d(\epsilon) \, d\epsilon, \tag{10} \]

where $\rho_d(\epsilon)$ is the $c_d$-level spectral density, $f(\epsilon)$ is the Fermi function,

\[ G_2 = \frac{2e^2}{\hbar c}, \tag{11} \]

is the quantum conductance with two spin channels,

\[ \Gamma_W = \frac{\pi \rho V^2}{1 + \pi^2 \rho^2 W^2}, \tag{12} \]

and

\[ \kappa = \frac{V_L V_R}{V^2}. \tag{13} \]

The asymmetry index $\kappa$ is a dimensionless factor that modulates the conductance. The modulus is unitary for symmetric couplings, $V_L = V_R$, and shrinks as the coupling asymmetry grows. To simplify the following theoretical analysis, we define the reduced conductance

\[ \bar{G} \equiv \frac{G}{\kappa}, \tag{14} \]

so that Eq. (10) reads

\[ \bar{G}(T) = \pi G_2 \Gamma_W \int \left( -\frac{\partial f}{\partial \epsilon} \right) \rho_d(\epsilon) \, d\epsilon. \tag{15} \]

### III. Characteristic Energies and Fixed Points

The spectral density $\rho_d$ is a function of energy and temperature. Since the Hamiltonian (6) is decoupled from the dot, we only have to diagonalize $H$ to compute $\rho_d$ and determine the conductance from Eq. (15). The computation is simple in special regimes, defined by the characteristic energies of the Hamiltonian.

In the absence of the potential $W$, the coupling to the leads broadens the dot level to the width

\[ \Gamma = \pi \rho V^2. \tag{16} \]

The potential $W$ reduces the broadening, as indicated by Eq. (12).
If the width \( \Gamma \) were zero, the dot occupation \( n_d \) would be conserved. The dynamics of the device would then be controlled by the eigenvalues \( E_d^\ell \) (\( \ell = 0, 1, 2 \)) of \( H_d \). The \( d^0 \) eigenstate would have energy \( E_d^0 = 0 \), the \( d^1 \) and \( d^2 \) eigenstates (where the subscript indicates the \( S_z \) eigenvalue) would have energy \( E_d^1 = V_G \), and the \( d^2 \) eigenstate would have energy \( E_d^2 = 2V_G + U \).

We are centrally interested in the gate-voltage range making \( E_d^1 \) smaller than \( E_d^0 \) and \( E_d^2 \), i.e., in the range \( 0 > V_G > -U \). In this interval, the dot acquires a magnetic moment \( \mu_B \). The interval is limited by the two \textit{charge-degeneracy points}, associated with voltages \( V_G^{0,-1} = 0 \) and \( V_G^{1,-2} = -U \). At the middle of the interval is the \textit{symmetric point}, attained when the gate voltage is \( V_G^1 = -U/2 \).

Without coupling, conduction would be impossible. With small coupling \( \Gamma_W \ll |V_G|, \Gamma_W \ll U \), charge transport is barred by an energy barrier \( \Delta E_c = \min\{||V_G|, U + V_G|\} \), except within a gate-voltage range of width \( \Gamma_W \) of either charge-degeneracy point. The barrier \( \Delta E_c \) is known as the \textit{Coulomb blockade}.

At moderately high temperatures, such that thermal energy \( k_BT \) lies in the interval \( \Delta E_c \gg k_BT \gg T_K \), the width \( \Gamma \) can be disregarded, the dot occupation is approximately conserved, and the Coulomb blockade controls the physics of conduction—the Coulomb blockade regime. Assuming that the width \( D \) of the conduction bands exceeds \( U \), we can see that the thermal energy is incommensurate with the other energy scales of the problem. Physically, the model Hamiltonian is then approximately equivalent to the \textit{local-moment fixed-point} Hamiltonian \( H^*_LM \) obtained by letting \( D, U \to \infty, V_G \to -\infty \), and \( \Gamma \to 0 \) in Eq. (7).

The local-moment fixed-point fixed-point Hamiltonian is equivalent to a dot with unitary occupation and magnetic moment \( \mu_B \) decoupled from conduction band of non-interacting electrons. The Hamiltonian reads

\[
H^*_LM = \sum_k \epsilon_k a_k^\dagger a_k + W f_0^\dagger f_0.
\]

(17)

where the superscript reminds us that the fixed-point Hamiltonian is devoid of characteristic energies.

\( H^*_LM \) is an idealized Hamiltonian whose many-body spectrum is approximately equal to the energy spectrum of the Hamiltonian \( H \) in the range \( \Delta E_c \gg \epsilon \gg \Gamma_W \). The dot level makes no contribution to the right-hand side. Still, the dot level has a spin-1/2 degree of freedom, which we will denote \( \vec{S} \).

The conduction band is phase shifted by the potential \( W \), i.e., each single-particle eigenstate acquires a phase shift \( \delta_w \), given by the expression

\[
\tan \delta_w = -\pi \rho W.
\]

(18)

Depending on \( W \), the phase shift can take any value in the interval \(-\pi/2 \leq \delta/2 \leq \pi/2 \). The LM fixed-point Hamiltonian can be visualized as a point with phase shift \( \delta \) along a line running from \(-\pi/2 \) to \( \pi/2 \).

### A. Kondo Hamiltonian

The fixed point is an idealization. In practice, neither \( U \), nor \( |V_G| \) are infinite. Even at (moderately) high temperatures, the Hamiltonian \( H \) is not exactly the fixed-point Hamiltonian. The high-energy many-body spectrum of \( H^*_LM \) is only an approximation to the spectrum of \( H \), because the finite Coulomb barriers allow virtual excitations to the \( d^0 \) and \( d^2 \) dot states.

The virtual excitations induce an antiferromagnetic coupling between the dot magnetic moment and the magnetic moments of the conduction electrons [25]. A more precise representation of the high-energy spectrum of \( H \) comes therefore from the equation

\[
H_K = \sum_k \epsilon_k a_k^\dagger a_k + W f_0^\dagger f_0 + J \vec{S} \cdot \sum_{\mu, \nu} \vec{\sigma}_{\mu \nu} f_0^\dagger \mu f_0^\nu. \tag{19}
\]

where the components of \( \vec{\sigma} \) are the Pauli matrices, and the coefficients of the second and third terms on the right-hand side are given by the Schrieffer-Wolff expressions [26]

\[
\rho \dot{W} = \rho W + \frac{\Gamma}{V_G} + \frac{\Gamma}{V_G + U}, \tag{20}
\]

and

\[
\rho J = \frac{\Gamma}{|V_G|} + \frac{\Gamma}{V_G + U}. \tag{21}
\]

Equation [19] defines the Kondo Hamiltonian. For thermal energies that are small in the scale of the Coulomb blockade, the spectra of \( H \) and \( H_K \) are approximately congruent. The right-hand sides of Eqs. [20] and [21] become very large in absolute value near the charge degeneracy points \( V_G = 0 \) and \( V_G = -U \).

Near the symmetric point, by contrast, as long as \( \Gamma \ll U \) there is a range of gate voltages such that \( \Gamma \ll |V_G| \) and \( \Gamma \ll U + V_G \). That gate-voltage range makes \( \rho J \ll 1 \) and places the device in the \textit{Kondo regime}.

The symmetric point lies at the middle of the Kondo regime. At the symmetric point, the second and third terms on the right-hand side of Eq. (20) cancel each other, and the phase shift equals \( \delta_w \). Elsewhere within the Kondo regime, the phase shift is given by the equality

\[
\tan \delta_0 = -\pi \left( \rho W + \frac{\Gamma}{V_G} + \frac{\Gamma}{V_G + U} \right). \tag{22}
\]

Physically, the phase shift is associated with the screening charge that forms in the vicinity of the \( f_0 \) orbital in response to the potential \( W \) and to the coupling to the quantum dot.
B. Frozen-level fixed point

If the device is cooled in the Kondo regime, at sufficiently low temperatures the antiferromagnetic interaction between the conduction electrons and the dot spin will induce the Kondo cloud. At temperatures well below the Kondo temperature, the dot spin will lock into a singlet with the conduction-electron spins, which will freeze the dot-spin degree of freedom.

As a result, at low thermal energies, with \( T \ll T_K \), the spectrum of \( H \) approaches that of the Hamiltonian obtained from Eq. (19) when we let \( J \to \infty \). The \( f_0 \) orbital then forms a singlet with the dot spin variable, and the Hamiltonian becomes equivalent to the quadratic form

\[
H_{FL} = \sum_k \bar{\epsilon}_k \bar{a}_k \bar{a}_k^\dagger + \tilde{W} \sum_{k,q} \bar{a}_k^\dagger \bar{a}_q,
\]

where the set of the conduction states \( \bar{a}_k \) and the localized orbital \( f_0 \) form an orthonormal basis that is complete relative to the original conduction states \( a_k \). The subscript on the left-hand side reminds us that the dot level is frozen, and the superscript, that \( H_{FL}^* \) is devoid of characteristic energies.

To be orthogonal to \( f_0 \), the new conduction states \( \bar{a}_k \) must deplete the region of the leads next to the quantum dot. They must therefore be phase-shifted by \( \pi/2 \) relative to the \( a_k \). It follows that the conduction energies \( \bar{\epsilon}_k \) are shifted relative to the \( \epsilon_k \):

\[
\rho \bar{\epsilon}_k = \rho \epsilon_k - \frac{1}{2},
\]

and that the FL fixed-point phase shift is

\[
\delta = \frac{\pi}{2} + \delta_0,
\]

where \( \delta_0 \) is the LM fixed-point phase shift.

C. Fixed-point conductances

To determine the conductance from Eq. (15), we must compute the spectral density \( \rho_d(\epsilon) \). An exact expression relates \( \rho_d(\epsilon) \) to the spectral densities of the linear combinations \( \sum_k a_k \) and \( \sum_k \epsilon_k a_k \) of the conduction operators \( \bar{c}_k \) [20, 27]. As the model Hamiltonian approaches a fixed point, the latter two spectral densities can be computed from the eigenvalues and eigenstates of the fixed-point Hamiltonian. The diagonalization of the fixed-point, single-particle Hamiltonians \( H_{FL}^* \) and \( H_{FL}^* \) is straightforward. It is therefore a simple matter to obtain the fixed-point spectral densities [29]

\[
\rho_d^* = \frac{1}{\pi T W} \sin^2(\delta_\epsilon - \delta_W) \quad (T \gg T_K \text{ or } T \ll T_K),
\]

where \( \delta_\epsilon \) denotes the fixed-point phase shift.

For \( W = 0 \), the phase shift \( \delta_W \) vanishes and we recover Langreth’s expression for the low-energy spectral density [28]. Equation (26) is not restricted to low energies. However, since the LM and the FL fixed points have distinct phase-shifts, the spectral densities at high and at low energies are different.

Substitution of the fixed-point results in Eq. (15) now yields the following expression for the fixed-point conductances:

\[
\tilde{G}^* = \tilde{G}_2 \sin^2(\delta_\epsilon - \delta_W). \quad (27)
\]

D. Thermal dependence of the conductance

If \( W = 0 \), the zero-bias conductance at the symmetric point is a universal function of the temperature scaled by the Kondo temperature [29, 30]:

\[
\tilde{G}(T) = \tilde{G}_2 G_S(T/T_K).
\]

Figure 2 displays the universal function \( G_S \) as a function of the ratio \( T/T_K \). The condition \( G_S(T = T_K) = G_2/2 \) defines the Kondo temperature. At high (low) temperatures, the Hamiltonian is close to the LM (FL) fixed point, and the conductance, close to zero \( (G_2) \). Physically, the coupling \( J \) between the dot and the conduction-electron spins is so weak that the dot moment is virtually decoupled from the leads. At the symmetric point the Coulomb blockade imposes the energy barrier \( \Delta E_c = U/2 \), much larger than the thermal energy. Conduction across the device is virtually impossible.

As the temperature is lowered, the Kondo cloud starts forming. As \( T \) drops past \( T_K \) the electrons within the cloud bind into a singlet with the dot electron. The binding is so tight that it allows ballistic transport.

![Universal function relating the SET conductance at the symmetric point \( V_G = -U/2 \) to the temperature scaled by the Kondo temperature.](image)

FIG. 2: Universal function relating the SET conductance at the symmetric point \( V_G = -U/2 \) to the temperature scaled by the Kondo temperature.
1. Particle-hole symmetry

The symmetric point is special. With $W = 0$ and $U = -V/2$, the Hamiltonian remains invariant under the particle-hole transformation

$$
egin{align*}
c_d &\rightarrow -c_d^\dagger; \\
c_k &\rightarrow c_q^\dagger.
\end{align*}
$$

Here, the momenta $k$ and $q$ are symmetric: given $k$, one chooses $q$ such that $q = -k$. The particle-hole transformation inverts the sign of the particle-hole transformation inverts the sign of the phase shift $\delta$. Consequently, the fixed-point phase shifts of the symmetric Hamiltonian can only be $\delta = 0$ or $\delta = \pi/2$. At the high-temperature (LM) fixed point the phase shift vanishes; at the low-temperature (FL) fixed point $\delta = \pi/2$. It follows from Eq. (27) that, at the symmetric point, $G_{LM} = 0$ and $G_{FL} = \pi/2$, as indicated by the high- and low-temperature limits in Fig. 2.

Instead, the conductance maps linearly onto the universal function $G(T/T_K)$.

At intermediate temperatures, the experimental conductance cannot follow the plot in Fig. 2, nor can it be proportional to $G_2(T/T_K)$.

In the Kondo regime, Eq. (35) is exact. It is instructive to compare it with the experimental data reported in Ref. [21] Equation (14), which relates the experimental conductance $G(T)$ to the reduced conductance $\tilde{G}(T)$, yields the following expressions for the high- and low-temperature limits of the experimental conductance:

$$
G_{LM} = \kappa G_2 \cos^2 \left( \frac{\pi n_d}{2} \right),
$$

and

$$
G_{FL} = \kappa G_2 \sin^2 \left( \frac{\pi n_d}{2} \right).
$$

At intermediate temperatures, the experimental conductance maps linearly onto the universal function. From Eq. (35) it follows that

$$
G \left( \frac{T}{T_K} \right) - \frac{G_2}{2} = \left( \frac{G_2}{2} - G_S \left( \frac{T}{T_K} \right) \right) \cos (\pi n_d).
$$
A. Experimental data

Grobis et al. \[21\] have measured the conductance of a single-electron transistor as a function of temperature, gate voltage, and bias voltage. We focus on their zero-bias results. To scan a Kondo plateau, the authors have accurately measured \(G\) on a \(V_G \times T\) grid comprising 34 uniformly spaced gate-voltages, ranging from \(-212.5\) mV to \(-196\) mV, and 17 temperatures, ranging from 13 mK to 205 mK. Figure 1(c) in Ref. \[21\] overviews the resulting data. At fixed gate-voltage, the conductance rises as the sample is cooled, from approximately \(0.5\mathcal{G}_2\) at \(T = 205\) mK to approximately \(0.85\mathcal{G}_2\) at \(T = 13\) mK. The rise is steeper at the middle of the plateau, around \(V_G = -205\) mV.

Qualitatively, we can see that Eq. \(38\) agrees with these features of the data. In fact, the agreement is quantitative, as illustrated by Fig. 3. Each panel plots the measured conductance \(G\) as a function of the universal conductance \(G_S\) for the depicted gate voltage. As long as the temperature is scaled by the Kondo temperature, we expect the relation between the two conductances to be linear.

Since \(T_K\) is unknown, we proceed by trial and error. The experimental temperatures are scaled by a trial Kondo temperature, and linear regression determines the optimum coefficient \(\kappa \cos(\pi n_d)\) and intercept \(\kappa \mathcal{G}_2/2\) fitting \(G(T/T_K)\) to \(G_S(T/T_K)\). If the linear correlation coefficient is sufficiently close to unity, we have found the Kondo temperature. Otherwise, we turn to Newton’s method for a better estimate of \(T_K\), and repeat the procedure. Convergence yields the Kondo temperature and the coefficients of the linear fit.

This procedure was applied to the thermal dependence of the conductance at each gate voltage in the experimental grid. In each case, the agreement was comparable to the fits in Fig. 3.

As the plots in Fig. 3 show, the straight lines can be extrapolated to the \(G_S \rightarrow \mathcal{G}_2\) (\(G_S \rightarrow 0\)) limit to yield the FL (LM) fixed-point conductance \(G_{FL}\) (\(G_{LM}\)). Linear regression therefore determines the high- and low-temperature limits of the conductance, which are inaccessible in the laboratory.

Figure 4 shows all \(34 \times 17 = 578\) experimental conductances, measured from \(G(T_K) = \mathcal{G}_2/2\), scaled by the difference \(G(0) - G(T_K)\) between the extrapolated low-temperature conductance and the Kondo-temperature conductance, as a function of the temperature scaled by \(T_K\). To identify the gate-voltage at which each conductance was measured, the inset shows the 34 Kondo temperatures as a function of \(V_G\). The near congruence between the symbols and the solid line representing the universal function scaled in the same fashion offers a measure of the overall harmony between the measurements and the expected universal behavior in the Kondo regime.

Figure 5 shows the resulting estimates of \(G_{FL}\) and \(G_{LM}\) as functions of the gate voltage. At each gate-voltage, the limit conductances determine the ground-state expectation value \(n_d\) of the dot occupancy and the
FIG. 5: (Color online) Fixed-point conductances \(G_{LM}\) and \(G_{FL}\) as functions of the gate voltage \(V_G\). At each gate voltage, the LM and FL fixed-point conductances result from extrapolating the \(G(T/T_K)\) vs. \(G_S(T/T_K)\) plots to \(G_S = 0\) and \(G_S = 1\), respectively, as illustrated by each panel in Fig. 4.

The deviation from \(\kappa = 1\) at high temperatures, in the Kondo regime, is universal. Other properties of the Anderson model, such as the mathematical connection between the physical features of the device and the LM Hamiltonian, are nonuniversal. The minimalist, inaccurate description of the physical features is responsible for the deviations.

We conclude that the Hamiltonian [1] cannot describe the device in Ref. [21] quantitatively. Given the simplicity of the model, which neglects electron-electron interactions within the leads, considers a single, structureless, half-filled conduction bands, adopts a single level to represent the quantum dot, and gives no attention to the spatial dependence of the potentials applied to the leads or to the momentum dependence of the couplings between the dot and the leads, the conclusion seems hardly surprising.

More puzzling is the contrast between the deviations of Fig. 6 from the expected behavior and the much superior agreements in Figs. 3 and 4. The puzzle, however, is easily solved. Recall that Eq. (29), besides exact in the Kondo regime, is universal. Other properties of the Anderson model, such as the mathematical connection between the physical features of the device and the LM Hamiltonian, are nonuniversal. The minimalistic, inaccurate description of the physical features is responsible for the deviations in Fig. 6 while universality protects the fits in Figs. 3 and 4 from such inaccuracies.

This underscores the call for ab initio treatments of the device. Consider, for definiteness, the experimental data by Grobis et al. [21]. While static DFT approaches may be unable to deal with the crossover from the LM to FL fixed points, even local approximations to the exchange-correlation functional should be sufficient to describe the LM fixed point and determine the LM conductance. Comparison with the solid blue circles in Fig. 5 would then test our understanding of the physics underlying the experimental data.

To examine the same argument from a different perspective, consider a local-density description of the LM fixed point associated with the model Hamiltonian \(H_{LM}\). \(H_{LM}\) is given by Eq. (17). Since the model conduction electrons are noninteracting, the exchange-correlation potential vanishes inside the leads. The Kohn-Sham eigenstates are the single-particle eigenstates of \(H_{LM}\).

DFT therefore yields the phase shift \(\delta = \delta_p\). From Eqs. (14) and (27), the conductance is predicted to vanish at high temperatures, in the Kondo regime. At the symmetric point, this agrees with the plot in Fig. 2. The prediction nonetheless disagrees, conspicuously, with the blue solid circles in Fig. 5.

DFT cannot be blamed for the disagreement. True, the local-density approximation neglects the antiferromagnetic interaction with the dot spin and hence misses the contribution from the last term on the right-hand side of Eq. (19) and the contribution to \(W\) from the last two terms on the right-hand side of Eq. (20). In the Kondo regime, however, those terms are small. They cannot account for the substantial conductances represented by the blue solid circles in Fig. 5.

The discrepancy is due to the shortcomings of the model, not to the limitations of the local-density approximation for the exchange-correlation functional. To strengthen the argument, we substitute \(\tilde{W}\) [given by Eq. (26)] for \(W\) on the right-hand side of Eq. (17). A
more accurate approximation results, which takes the spin-independent phase shift induced by dot moment into account. Notwithstanding the improvement, the resulting conductance is still zero at the symmetric point, which corresponds to $V_G \approx -205 \text{ mV}$ in the experimental setup [21].

The model fails to account for the relatively large LM conductances resultant from the extrapolations of the experimental data. A more detailed description of the experimental device, based on *ab initio* computations, is necessary to describe the LM fixed point.

**V. SUMMARY**

The single-electron transistor poses a concrete challenge to DFT. Recent progress, backed by improved local approximations for the exchange-correlation functional especially designed to yield the correct density derivative, have yielded accurate descriptions of the ground-state conductance for the Anderson Hamiltonian. Unfortunately, this approach has only been proven successful in the region where it must give satisfactory results by construction [18, 32].

To propose an alternative static approach, we have combined concepts drawn from renormalization-group theory with the notion that the thermal dependence of the SET conductance is parametrized by the ground-state expectation value for the quantum-dot occupation. Chiefly important in this context is the progressive formation of the screening cloud in the Kondo regime as the Hamiltonian crosses over from a high- to a low-energy fixed points. At high temperatures, the dot possesses a magnetic moment. At low temperatures, the dot spin forms a singlet with the conduction electrons.

Renormalization-group theory associates the high-energy spectrum of the Anderson Hamiltonian with the many-body spectrum of the local-moment fixed-point Hamiltonian $H_{LM}^*$, and the low-energy spectrum with that of the frozen-level fixed-point $H_{FL}^*$. At intermediate energies, which correspond to the temperature range over which the dot magnetic moment is screened, the model Hamiltonian crosses over from the vicinity of $H_{LM}^*$ to the vicinity of $H_{FL}^*$.

The physical properties describing the SET crossover are universal. In particular, as discussed in Section III, the electrical conductance maps linearly onto a universal function of the temperature scaled by the dot temperature $T_K$. The mapping is controlled by the dot occupancy $n_d$.

The linear mapping fits the experimental data by Grobis et al. [21] with very small deviations. Nonetheless, the resulting dot occupancies $n_d$ are substantially lower than unity, and the asymmetry index of the device $\kappa$ is gate-voltage dependent and exceeds unity.

The thermal dependence of the conductance for the Anderson model in the Kondo regime reproduces the experimental data very well, while non-universal aspects of the same model offer a blurred picture of the SET constructed by Grobis et al. [21]. *Ab initio* treatment of the device is therefore necessary before quantitative description of the experimental data becomes possible. Given that universality simplifies the description of the crossover from the high- to the low-temperature fixed points, *ab initio* description of the high-energy fixed point will suffice.

From a practical viewpoint, this is convenient, for in contrast with the crossover the high-energy region yields to perturbative treatment [22]. Moreover, the high-energy fixed point having no characteristic energy scales, its properties are temperature independent. The ground-state energy of $H_{LM}^*$ can therefore be computed by standard DFT methods.

By contrast, the crossover to the FL fixed point calls for special, non-perturbative mathematical procedures. In this context, only the the Bethe-Ansatz [33] and the numerical renormalization-group [20, 29, 30] approaches have yielded exact or essentially exact results. The remaining challenge is to adapt one of those two methods, so that the DFT treatment of the high-energy spectrum can serve as input for the non-perturbative description of the crossover. Current work is addressing that problem [33].

**VI. ACKNOWLEDGMENTS**

Three decades ago, Hardy Gross showed the ropes of DFT to one of us (LNO). In exchange, he requested a talk on the Kondo problem, which was never materialized. So here it is, Hardy, at long last. Too little, and too late, but drawn from the heart, in memory of the grand time. Close your eyes, for a second, and you may see Walter and the two of us gathered around his table, lit by the setting sun and a hundred flickering rays coming from the blue waters of the Pacific. Thanks for those moments, and for all that I have learned from you. Live long, Hardy, and leads us farther.

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