

Charge dynamics and Kondo effect in single-electron traps in field-effect transistors

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We study magnetoelectric properties of single-electron traps in metal-oxide-semiconductor field-effect transistors. Using a microscopic description of the system based on the single-site Anderson-Holstein model, we derive an effective low-energy action for the system. The behavior of the system is characterized by simultaneous polaron tunneling (corresponding to the charging and discharging of the trap) and Kondo screening of the trap spin in the singly occupied state. Hence, the obtained state of the system is a hybrid between the Kondo regime, typically associated with single-electron occupancy, and the mixed-valence regime, associated with large charge fluctuations. In the presence of a strong magnetic field, we demonstrate that the system is equivalent to a two-level system coupled to an ohmic bath, with a bias controlled by the applied magnetic field. Due to the Kondo screening, the effect of the magnetic field is significantly suppressed in the singly occupied state. We claim that this suppression can be responsible for the experimentally observed anomalous magnetic-field dependence of the average trap occupancy in Si—SiO₂ field effect transistors.

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I. INTRODUCTION

Experimental techniques probing dynamics of a few state quantum systems have been of great interest recently as they may provide prospects for the development of electronics and computing. Examples of such systems and techniques in solid state include quantum dots,¹ superconducting qubits,² magnetic resonant force microscopy,³ and single-electron traps in a metal-oxide-semiconductor field-effect transistor (MOSFET).⁴⁻⁸

This latter system, which is a subject of this work, consists of a defect located near the oxide-semiconductor interface of a MOSFET [Fig. 1(a)]. The tunneling between the defect and the two-dimensional electron gas (2DEG) in a MOSFET inversion layer manifests itself as a random telegraph signal (RTS) in the transport current through the MOSFET. When a certain trap energy level (whose energy can be controlled by the gate voltage) crosses the chemical potential of the 2DEG, electrons can hop between the level and the conduction channel, thus charging and discharging the trap. For a sufficiently small MOSFET this leads to the sudden switching in the resistivity of the conduction channel and hence to RTS in the transport current.

The charge dynamics of the trap exhibits a number of features consistent with dynamics of a two-level system (TLS) coupled to an ohmic environment.⁵ In particular, the experimental dependence of tunnel rates on the TLS bias (controlled by the gate voltage) and external temperature was found to agree with those calculated for the spin-boson Hamiltonian.⁹ However there are a number of RTS properties that cannot be explained based on the TLS phenomenology.

First of all, the RTS is observed to occur on a relatively large, millisecond-to-second time scale, which seems to indicate that the observed traps are positioned sufficiently far, at distances 20–25 Å from the 2DEG. At the same time, the direct electrostatic measurements of trap positions indicate that this is usually not the case—the traps are located only a few angstroms from the inversion layer.⁸

Another aspect that clearly lies outside the scope of TLS phenomenology has recently been revealed in the experi-

ments by Xiao *et al.*,⁷ where the dependence of the RTS on an applied magnetic field was studied. In these experiments, from the gate voltage and the magnetic-field dependence of RTS, it was determined that the most likely origin of RTS was the random switching between (spin- $\frac{1}{2}$, neutral) and (spin-0, negatively charged) states of the trap. In particular, at sufficiently high temperatures (above several degrees Kelvin), the relative probability of the empty state of the trap to the filled state was rapidly increasing with the applied magnetic field, consistent with the simple model expectation $P_1/P_2 \propto \exp(g\mu_B B/2T)$.⁷ However, at lower temperatures significant deviations from the simple paramagnetic behavior was observed, possibly indicating quenching of trap's magnetic moment.⁷ Such magnetic behavior appears to be consistent with the Kondo effect.

However, it is well known that the Kondo screening is only effective for sufficiently strong hybridization of the localized state with the continuum. Given the extremely slow observed tunnel rate, one should conclude that the Kondo temperature should be negligibly small, thus ruling out the possibility of the Kondo effect explanation.

The purpose of this work is to show that the slow charge dynamics and the Kondo effect are, in fact, *not* mutually exclusive, if we take into account the strong electron-optical phonon coupling in the oxide layer of a Si MOSFET. In our previous work¹⁰ we have proposed that this coupling is the likely origin of exponential renormalization in RTS time-scales and can explain the inconsistency between expected and observed positions of traps. In the present work, starting from the microscopic description of the system based on the Anderson-Holstein model, we derive an effective low-energy action for the charge *and spin* dynamics of the trap. We find that the low-temperature behavior of the system is characterized by simultaneous polaron tunneling (corresponding to the charging and discharging of the trap) and Kondo screening of the trap spin in the singly occupied state. It is crucial that the Kondo temperature need not be small as it is controlled by the *bare* hybridization matrix element between the localized

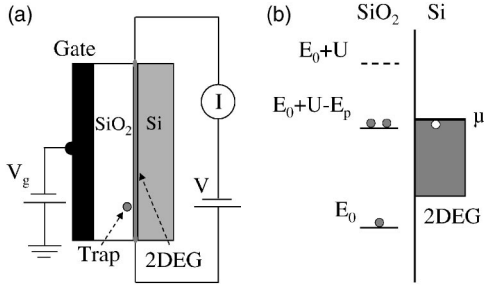


FIG. 1. (a) Schematics of traps in MOSFETs and (b) a diagram for the trap energy levels. Coupling to optical phonons shifts the twice-occupied level.

and conduction electrons, i.e., it is not affected by the polaronic slowdown. The simple explanation is related to the fact that although the real charge tunneling is suppressed by the polaronic effect, the virtual tunneling processes that lead to the local moment-conduction electron spin-exchange interaction need not be affected by this renormalization. In particular, if the on-site Coulomb interaction (which essentially determines the inverse timescale for the virtual processes) is larger than the phonon frequency, the lattice does not have time to react to these processes. As a result, the spin transitions in the trap are not affected by the presence of the oscillator and thus the Kondo timescale depends on the bare tunneling rate γ_T^0 rather than the renormalized one γ_T .

In the presence of a strong magnetic field, we map our system onto a two level-level system (TLS) strongly coupled to an ohmic bath, with a bias controlled by the applied magnetic field. Due to the Kondo screening, the bias introduced by the magnetic field is significantly suppressed compared to the bare Zeeman energy. We claim that this suppression can be responsible for the experimentally observed⁷ anomalous magnetic-field dependence of the average trap occupancy in Si—SiO₂ field-effect transistors.

Similar polaronic renormalizations have been considered earlier in the context of molecular crystals¹¹ and magnetic dielectrics.¹² More recently, related Hubbard-Holstein models have been applied to heavy fermion compounds to study electron-lattice effects, including valence instabilities.^{13,14}

II. MODEL

To describe the electronic part of the trap-channel system we use the Anderson-Hamiltonian

$$H_A = \sum_{k\sigma} E_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} E_0 d_{\sigma}^\dagger d_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{k\sigma} T_{cd} (c_{k\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{k\sigma}), \quad (1)$$

where $c_{k\sigma}^\dagger$ ($c_{k\sigma}$) and d_{σ}^\dagger (d_{σ}) are creation(annihilation) operators of electrons in the conduction band and at the localized defect orbitals, respectively, $n_{\sigma} = d_{\sigma}^\dagger d_{\sigma}$ ($\sigma = \uparrow, \downarrow$). U and T_{cd} are the on-site Coulomb energy and the hybridization matrix element, respectively. The coupling strength between the localized states and the 2DEG can be characterized by $\Gamma = \pi \nu T_{cd}^2$, where ν is the density of states in the 2DEG. The

single particle level of the trap is assumed to be positioned deep below the chemical potential of 2DEG, $E_0 < \mu$, as shown in Fig. 1(b). For simplicity we will assume that the conduction band is symmetric and set $\mu = 0$.

Another interaction that we include in our model is due to optical phonons in the Si MOSFET oxide layer. SiO₂ is a polar crystal and known to exhibit strong electron-optical phonon coupling leading to formation of polaronic states. We incorporate this electron-phonon coupling in our model as

$$H = H_A + \lambda \left(\sum_{\sigma} n_{\sigma} - 1 \right) \hat{x} + \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2 \hat{x}^2}{2}. \quad (2)$$

Here x and p are displacement and conjugate momentum of local optical phonon of frequency ω_0 ($\omega_0 \sim 50$ meV at Si—SiO₂ interface), m is the phonon effective mass (of the order of SiO₂ crystal unit cell mass), and λ is the coupling constant between the excess charge in the trap and the phonon. We assume the trap state with one electron is neutral and, therefore, introduce the off-setting -1 term in the electron-phonon interaction in Eq. (2). The strength of the electron-phonon coupling has been estimated in Ref. 10 and can be expressed in terms of the polaronic shift $E_p = \lambda^2 / 2m\omega_0^2 \sim 1$ eV. In the following we will assume that $U \gg E_p \gg \Gamma > \omega_0$.

III. EFFECTIVE ACTION

We analyze low-temperature partition function of the system $\mathcal{Z} = \text{Tr}[\exp(-\beta H)]$, where H is given by Eq. (2) and β^{-1} is smaller than any energy scale in the system. It is convenient to decouple the U term in Hamiltonian (1) by means of the Hubbard-Stratanovich transformation by writing the spin-spin interaction as $U n_{\uparrow} n_{\downarrow} = -(U/2)(n_{\uparrow} - n_{\downarrow})^2 + (U/2)(n_{\uparrow} + n_{\downarrow})$.¹⁵ The partition function can be then cast in the functional integral form as

$$\mathcal{Z} = \int \mathcal{D}X \mathcal{D}Y \exp - \int_0^{\beta} d\tau \left[\frac{M\dot{X}^2}{2} + \frac{(X - \Delta)^2}{4E_p} + \frac{Y^2}{2U} \right] \times \langle \mathcal{T} e^{-\int_0^{\beta} d\tau H_{\uparrow}[X(\tau) + Y(\tau)]} \rangle \langle \mathcal{T} e^{-\int_0^{\beta} d\tau H_{\downarrow}[X(\tau) - Y(\tau)]} \rangle, \quad (3)$$

where $H_{\sigma}[Z(\tau)] = Z(\tau) d_{\sigma}^{\dagger}(\tau) d_{\sigma}(\tau)$ and $\Delta = E_0 + (U/2) + 2E_p$. Here the explicit “time” dependence of $d_{\sigma}^{\dagger}(d_{\sigma})$ is defined by the interaction representation with respect to kinetic plus tunneling terms in the Hamiltonian (1). In Eq. (3) we have introduced $X = \lambda x + E_0 + (U/2)$ as a coordinate of the oscillator in units of energy and $M = m/\lambda^2$ as the oscillator’s mass in the corresponding units. The scalar field Y is conjugate to the spin of the trap, \mathcal{T} stands for time ordering, and the angular brackets denote averaging with respect to electronic degrees of freedom. The averaging of the ordered exponents in Eq. (3) can be done by following the prescription of Refs. 16 and 17 based on the theory of singular integral equations. Here we provide the result: the functional integral in Eq. (3) can be cast in the form $\mathcal{Z} = \int \mathcal{D}[X, Y] \exp[-\int_0^{\beta} d\tau (\mathcal{V} + \mathcal{K})]$, where functionals \mathcal{V} and \mathcal{K} represent potential and kinetic energy of a particle moving in a two-dimensional (X, Y) plane

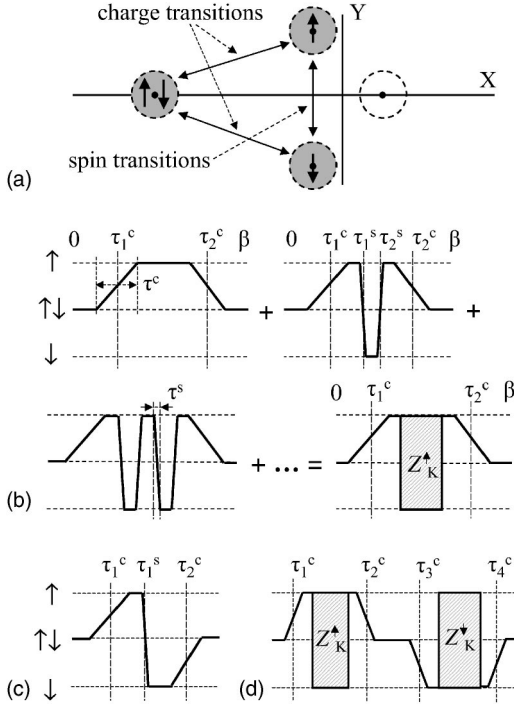


FIG. 2. (a) Local minima for the effective potential in Eq. (4b); (b) a classical path contributing to the transition amplitude between a two-electron and a spin-up electron state; and (c) example of a path containing a spin-kink “monopole.” Such trajectories do not contribute to the transition amplitudes; (d) trajectory that involves multiple charge-kinks.

$$\mathcal{V} = \frac{(X - \Delta)^2}{4E_p} + \frac{Y^2}{2U} + V(X + Y) + V(X - Y),$$

$$V(Z) = \frac{Z}{2} - \frac{Z}{\pi} \tan^{-1}\left(\frac{Z}{\Gamma}\right) + \frac{\Gamma}{2\pi} \log\left[1 + \left(\frac{Z}{\Gamma}\right)^2\right]; \quad (4a)$$

$$\mathcal{K} = \frac{M\dot{X}^2}{2} + K(X + Y) + K(X - Y),$$

$$K(Z) = \frac{1}{\pi^2} \int_0^\tau d\tau' \log(\tau - \tau') \frac{dZ(\tau')}{d\tau'} \frac{d}{d\tau} \times \left[\frac{Z(\tau)}{Z^2(\tau) - Z^2(\tau')} \log \frac{\Gamma^2 + Z^2(\tau)}{\Gamma^2 + Z^2(\tau')} \right]. \quad (4b)$$

The potential energy of the “particle” is presented in Fig. 2(a). It has four local minima. The two minima on the X-axis (at $X_2 = \Delta - 4E_p$ and $X_0 = \Delta$ for $U, E_p \gg \Gamma$) correspond to different charge occupations of the trap, i.e., by two and by zero electrons. Up to an additive constant [which we have dropped in Eq. (3)] potential energies of these minima are $\mathcal{V}_2 = 2E_0 + U - E_p$ and $\mathcal{V}_0 = -E_p$. The two minima off the X-axis (at $X_\uparrow = \Delta - 2E_p$, $Y_\uparrow = U$, and $X_\downarrow = \Delta - 2E_p$, $Y_\downarrow = -U$) are degenerate in the absence of external magnetic field with $\mathcal{V}_\uparrow = \mathcal{V}_\downarrow = E_0$ and obviously correspond to the occupation of the trap by one electron with up- and down-spin, respectively. As can be seen directly from Hamiltonians (1) and (2),

the minima can be interpreted as zero-temperature free energies of the trap occupied by two, zero, and one electrons in the limit of vanishingly small Γ . In the RTS experiments the traps are filled with either one or two electrons,⁷ and therefore we assume that $\mathcal{V}_\uparrow \approx \mathcal{V}_\downarrow \approx \mathcal{V}_2 < \mathcal{V}_0$ (or $E_0 \approx 2E_0 + U - E_p < -E_p$).

IV. EVALUATION OF FUNCTIONAL

The kinetic part of the energy in Eq. (4) will force the particle to tunnel between the minima. Because the energy of the empty state [denoted by the blank circle in Fig. 2(a)] is greater than that for the other three states (the shaded minima in Fig. 2), it will be effectively decoupled from those states. [Transition amplitudes to the empty state will contain exponentially small prefactors $\exp(-\beta(\mathcal{V}_0 - \mathcal{V}_2)) \ll 1$.] An example of the “classical” trajectory for a transition between the two-electron state and spin-up state is presented in Fig. 2(b). Let us first write down explicitly the transition amplitude that corresponds to the first diagram in Fig. 2(b). In doing so we must, in principle, determine the classical trajectory for the effective action given by Eq. (4) between the two local minima corresponding to the singlet and spin-up states. Solving the resulting classical equation of motion, however, is difficult. Instead we approximate the classical path by a piecewise linear kink trajectory, as shown in Fig. 2(b).^{16,17} Duration of each “charge” kink (i.e., transition between the two-electron state and a one-electron state), which we denote by τ^c , can be determined by minimizing the effective action for a single linear kink trajectory with respect to τ^c . Upon substitution of such linearized trajectory in Eq. (4) the transition amplitude of interest can be written as

$$\xi_c^2 \int_0^\beta \frac{d\tau_2^c}{\tau^c} \int_0^{\tau_2^c} \frac{d\tau_1^c}{\tau^c} e^{\delta_c(\tau_1^c - \tau_2^c) - \alpha_c \log[(\tau_2^c - \tau_1^c)/\tau^c]}, \quad (5)$$

where parameters ξ_c , α_c , and τ^c are

$$\alpha_c = \left(\frac{2}{\pi} \tan^{-1} \frac{U}{\Gamma}\right)^2, \quad (6a)$$

$$\xi_c = \left(\frac{\Gamma}{U}\right)^{1/2} \exp\left(-\frac{2E_p}{\tau^c \omega_0^2}\right), \quad (6b)$$

$$\tau^c \approx \frac{\sqrt{6}}{\omega_0}. \quad (6c)$$

In the above expression for the transition amplitude the kinks at time moments τ_1^c and τ_2^c interact logarithmically and α_c is the dimensionless coupling strength. The fugacity ξ_c , which is essentially the probability for a kink to occur at a given time, is suppressed by an exponentially small quantity in Eq. (6b) as a consequence of the oscillator having a finite mass. This suppression of charge tunneling is in agreement with the our previous result,¹⁰ where we argued that the inconsistency between the observed and expected tunnel rates in the RTS systems is due to the presence of a local phonon strongly coupled to the trap charge. The quantity δ_c in the above equation is a bias between one- and two-electron states, $\delta_c = \mathcal{V}_2 - \mathcal{V}_{\uparrow,\downarrow} = E_0 + U - E_p$.

Next let us look at the transition amplitude that involves spin transitions. In Fig. 2(b) this amplitude can be singled out as an effective self-energy part of the diagrams that involve $2n$ ($n=0,1,\dots$) kinks and antikinks. Applying the same procedure, i.e., assuming that all the trajectories are piecewise linear, evaluating their contribution to the effective action in Eq. (4), and minimizing the action with respect to the width of the spin kinks τ^s , we obtain that the spin-transition amplitude, Z_K^σ in Fig. 2(b), is given by

$$\begin{aligned} Z_K^\sigma(\tau_2^c - \tau_1^c) &= \sum_n \xi_s^{2n} \int_{\tau_1^c}^{\tau_2^c} \frac{d\tau_{2n}^s}{\tau^s} \dots \int_{\tau_1^c}^{\tau_2^c} \frac{d\tau_2^s}{\tau^s} \int_{\tau_1^c}^{\tau_2^c} \frac{d\tau_1^s}{\tau^s} \\ &\times \exp \left[-\sigma \delta_s \sum_i (-1)^i \tau_i^s + \frac{\sigma \delta_s \beta}{2} \right] \\ &\times \exp \left[\alpha_s \sum_{j>k}^{2n} (-1)^{j-k} \log \frac{\tau_j^s - \tau_k^s}{\tau^s} \right] \end{aligned} \quad (7)$$

$$\alpha_s = 2 \left(\frac{2}{\pi} \tan^{-1} \frac{U}{\Gamma} \right)^2, \quad (8a)$$

$$\xi_s = \frac{\Gamma}{U}, \quad (8b)$$

$$\tau^s \approx \frac{3\alpha_s}{U} \approx \frac{6}{U}. \quad (8c)$$

Here, $\delta_s = g\mu_B B$ is the energy splitting between the bare spin-down and spin-up states because of the applied magnetic field B .¹⁸ The transition amplitude Z_K^σ in Eq. (7) is of the same form as the grand partition function of a Coulomb gas of plus or minus kinks positioned along a straight line of length $\langle \tau_2^c - \tau_1^c \rangle$ interacting logarithmically with the coupling strength α_s and chemical potential defined as $e^{-\mu} = \xi_s$.¹⁹ In order to evaluate the full transition amplitude in Fig. 2(b) we must, in principle, take into account that the charge kinks at the ends of the interval, i.e., at “positions” τ_1^c and τ_2^c , interact [also logarithmically, as can be seen from the effective action in Eq. (4)] with the spin kinks at positions τ_j^s . One can see, however, that this interaction is effectively weak. Indeed, kinks at τ_j^s are coupled strongly with each other and tend to form close pairs (dipoles) of average effective “size” of the order $d \sim \tau^s / (2 - \alpha_s) \sim 1/\Gamma$, whereas the dipoles are separated, on average, by distances of the order of $l \sim \tau^s / \xi_s^2 \sim U/\Gamma^2$.¹⁹ The kinks at τ_i^c are separated from those at τ_j^s by a distance (time) at least of the order $\tau^c \sim 1/\omega_0$, which physically represents the time needed for the formation of the dressed electron-phonon state in the trap. Thus, the interaction energy for a kink at τ_1^c with a dipole at $\tau_1^c + \tau$ is of the order d/τ . Summing over the dipoles (with the closest dipole located at distance of the order τ^c from the charge kink at τ_1^c and the farthest dipole roughly at τ_2^c) one finds that the charge kink-dipole interaction energy for the transition amplitude in Fig. 2(b) is $\sim (d/l) \int_{\tau_1^c}^{\tau_2^c} d\tau / \tau \sim (\Gamma/U) \log[(\tau_2^c - \tau_1^c)/\tau^c]$. This interaction is of the same long-range form as that between the kinks at τ_1^c and τ_1^s [e.g., Eq. (5)], however,

parametrically it is much weaker, $\alpha_c \sim 1 \gg (\Gamma/U)$. Therefore, interaction between the charge kinks and the spin kinks can be neglected. Also, we do not need to consider configurations with an odd number of spin kinks between the charge kinks [e.g., Fig. 2(c)]. That is because the energy of an unpaired kink diverges logarithmically with $\langle \tau_2^c - \tau_1^c \rangle$, and hence its formation is not favorable. Thus the transition amplitude that contains two charge kinks at $\tau_{1,2}^c$ can be written as

$$\xi_c^2 \int_0^\beta \frac{d\tau_2^c}{\tau^c} \int_0^{\tau_2^c} \frac{d\tau_1^c}{\tau^c} Z_K(\tau_2^c - \tau_1^c) e^{\delta_c(\tau_1^c - \tau_2^c) - \alpha_c \log[(\tau_2^c - \tau_1^c)/\tau^c]},$$

where $Z_K = Z_K^\uparrow + Z_K^\downarrow$.

We are now ready to extend this expression to a higher-order amplitudes. One such amplitude with four charge kinks at τ_j^c is shown in Fig. 2(d). We note that only charge kinks connecting the singlet state with the *same* spin state interact. Hence, we assign superscript σ to distinguish between different types of charge kinks, $\tau_j^c \rightarrow \tau_j^{\sigma j}$. Using the same energetic arguments as before, we can show that the interaction between the spin kinks in different domains, as well as the interaction between any charge kinks and spin kinks, is negligible. Therefore, the transition amplitude can be written as

$$\begin{aligned} Z &= \sum_{n, \sigma_{2j} = \sigma_{2j-1} = \pm 1} \xi_c^{2n} \int_0^\beta \frac{d\tau_{2n}^{\sigma_{2n}}}{\tau^c} \dots \int_0^{\tau_2^{\sigma_2}} \frac{d\tau_1^{\sigma_1}}{\tau^c} \\ &\times \prod_{j=1}^n Z_K^{\sigma_{2j}}(\tau_{2j}^{\sigma_{2j}} - \tau_{2j-1}^{\sigma_{2j-1}}) \exp \left[-\delta_c \sum_{j=1}^{2n} (-1)^j \tau_j^{\sigma_j} \right] \\ &\times \exp \left[\alpha_c \sum_{j>k}^{2n} (-1)^{j-k} \delta_{\sigma_j, \sigma_k} \log \frac{\tau_j^{\sigma_j} - \tau_k^{\sigma_k}}{\tau^c} \right]. \end{aligned} \quad (9)$$

In zero magnetic field ($\delta_s=0$), the spin partition function $Z_K^\uparrow(\tau - \tau') = Z_K^\downarrow(\tau - \tau') \sim \exp[-(\tau - \tau')F_0]$, where F_0 is the free energy per unit length for the Coulomb gas described by the classical partition function of Eq. (7). In this regime, the full partition function of Eq. (9) corresponds to a gas of charges of *two flavors*, with charges at points τ_{2j} and τ_{2j-1} having the same flavor and opposite charge, and only charges of the same flavor interacting with each other. In the presence of applied magnetic field, the symmetry between the two flavors is broken.

V. MAGNETIC-FIELD DEPENDENCE

To evaluate the effect of magnetic field on partition function Eq. (9), we first determine the dependence of Z_K^σ on magnetic field. For that we use the scaling procedure for the Coulomb gas due to Anderson *et al.*¹⁹ The renormalization group equations read

$$\frac{d\alpha_s}{d \log \tau^s} = -4\alpha_s \xi_s^2 + O(\xi_s^3), \quad (10a)$$

$$\frac{d\xi_s}{d \log \tau^s} = \frac{1}{2} \xi_s (2 - \alpha_s) + O(\xi_s^4), \quad (10b)$$

$$\frac{d(\delta_s \tau^s)}{d \log \tau^s} = (1 - 2\xi_s^2) \delta_s \tau^s + O(\xi_s^4), \quad (10c)$$

$$\mathcal{Z}_K[(\beta/\tau^s), \xi_s, \alpha_s] = \exp(\beta\Delta F) \mathcal{Z}_K[(\beta/\tilde{\tau}), \tilde{\xi}_s, \tilde{\alpha}_s]. \quad (10d)$$

where $\Delta F = \int_{\tilde{\tau}}^{\tau} d \log \tau' \xi_s^2 / \tau'^s$. For sufficiently strong magnetic field, ($\delta_s > T_K = \tau^{s-1} \exp[-1/\xi_s]$), the scaling should be terminated when $\tilde{\delta}_s \tilde{\tau} \sim 1$. At this point the magnetic field becomes very strong (on the renormalized energy scale), whereas the long-range coupling constant α_s decreases and so the system moves away from the quantum phase transition point at $\alpha_s = 2$ into the disordered phase.¹⁹ In the symmetric case ($2 - \alpha_s = 4\xi_s$) relevant here, the scaling Eqs. (10b) and (10c) coincide (up to quadratic terms in ξ_s and $2 - \alpha_s$) and can be easily solved analytically. For $\xi_s \ll 1$ the resulting renormalized $\tilde{\delta}_s$ and $\tilde{\xi}_s$ are

$$\tilde{\delta}_s = \delta_s \exp[-(1/2)\log^{-1}(\delta_s/T_K) + O(\xi_s)], \quad (11a)$$

$$\tilde{\xi}_s = \log^{-1}(\delta_s/T_K) + O[\log^{-3}(\delta_s/T_K)]. \quad (11b)$$

It is easy to see that in the rescaled system the long-range coupling becomes irrelevant. A simple perturbative estimate for the average size of a dipole is $\tilde{\tau}/(\tilde{\delta}_s \tilde{\tau})^2 \sim \tilde{\tau}$ and therefore both intra- and interdipole interactions are negligible. \mathcal{Z}_K can then be readily summed by means of Laplace transform¹⁰ with a simple result

$$\begin{aligned} \mathcal{Z}_K^\uparrow(\tau) &= \exp(\tau\{F'_0 + \tilde{\delta}_s + O[\log^{-3}(\delta_s/T_K)]\}), \\ \mathcal{Z}_K^\downarrow(\tau) &\approx \xi_s^2 \exp\{\tau\{F'_0 + \tilde{\delta}_s\}\} + \exp\{\tau\{F'_0 - \tilde{\delta}_s\}\}, \end{aligned} \quad (12)$$

where F'_0 is magnetic-field-independent free energy and $\tilde{\delta}_s$ is given by Eq. (11). In the long-time (low-temperature) limit that we are interested in, \mathcal{Z}_K^\downarrow is negligible compared to \mathcal{Z}_K^\uparrow . Hence, in the partition function [Eq. (9)] only the kinks that correspond to the transition between the singlet and the *dressed* spin-up states survive. The partition function becomes then equivalent to the one for a two-level system coupled to an ohmic bath.⁹ Equation (12) together with Eq. (9) indicates that an external magnetic field introduces an effective bias for the TLS. This bias, however, is significantly reduced [see Eq. (11)] as compared to the bare Zeeman energy of a paramagnetic spin. This suppression results from the interaction between the spin kinks in partition function Eq. (7) and corresponds to the Kondo effect.^{19,9} Indeed, the magnetization in the singly occupied state can be easily computed as $M \approx \partial \tilde{\delta}_s / \partial (g\mu_B B) = \frac{1}{2}(1 - 1/[2 \log(g\mu_B B/T_K)])$, consistent with the Bethe ansatz result of Andrei *et al.*²⁰

It is important that the Kondo energy scale T_K is *not* determined by the extremely slow charge tunneling rate (of the order of ξ_s^2/τ^s). Rather, the fugacity ξ_s , which determines T_K in Eq. (12), is because of virtual transitions between Fermi sea and the localized orbital. In the language of the effective action in Eq. (4) these virtual transitions correspond to tunneling of the Y field, which, unlike the X field, is massless. Therefore, as can be seen from Eq. (7), the fugacity ξ_s does not contain the exponentially small quasiclassical suppression factor corresponding to the ‘‘penetration under the barrier,’’ which strongly reduces the charge fugacity ξ_c [Eq. (6)]. As a result the Kondo temperature ($\sim \exp[-1/\xi_s]$) can be

quite large leading to significant renormalization of the magnetic-field-induced TLS bias.

VI. DISCUSSION AND CONCLUSIONS

In this work we considered an interplay between magnetism and the lattice effects in for a single Anderson impurity coupled to a continuum. We have found that even for extremely slow electron tunneling between the continuum and the localized orbitals, a significant exchange interaction between the conduction and the impurity electrons may exist. This is unusual since in the standard Anderson impurity case the exchange interaction is proportional to the localized level width. That is because only the real charge tunneling processes are affected by the polaronic renormalization, but the fast virtual processes that cause the exchange interaction are not.

The effective action for the model that we find is equivalent to the well-known Kondo (or s - d) model for the single defect occupancy, but with additional tunneling terms that connect the single occupancy sector to the other (zero or double) occupancy sectors. Indeed, this connection can be formally established by integrating out the phonon degrees of freedom (see the Appendix). It was earlier found that such a generalized Anderson model can exhibit both spin and charge Kondo effects.²¹ In the regime of weak residual hybridization that we considered here, only the spin-Kondo effect is relevant.

Based on the above presented arguments, we argue that the anomalously weak magnetic-field dependence of the interface trap occupancy observed in the low-temperature experiments of Xiao *et al.* can be explained by the Kondo screening of the local moment in the singly occupied state of the trap, assuming that the Kondo temperature is $T_K \sim 1$ K. Then, for low temperatures, $T < T_K$, we expect that the ratio of the probabilities corresponding to single and double occupancies of the trap should scale as $P_1/P_2 \propto \exp(g\mu_B \tilde{B}/2T)$, where the effective magnetic field \tilde{B} is related to the applied magnetic field B as $\tilde{B} = B \exp(-1/[2 \log(g\mu_B B/T_K)])$ for $g\mu_B B > T_K$.

Further detailed experimental study is necessary to test out the theoretical picture for the Kondo effect in the electrically active defects (traps) in Si field-effect transistors. It is worth noting, however, that similar physics, i.e., simultaneous slow charge dynamics and the Kondo effect, is expected to occur in any other system that has defects located at the interface between a strongly polar insulator and a conductor. One possible way to detect the Kondo effect is to look for low-temperature anomalies in the FET channel resistivity. Another approach is to look for spectral features (Kondo peak) by direct tunneling through a defect at the SiO₂-Si interface.

In summary, we have derived an effective action for the charge dynamics in a single electron trap in a Si MOSFET and have shown that in the limit of a strong magnetic field ($g\mu_B B > T_K$) it is equivalent to a two-level system strongly coupled to an ohmic environment. The effective bias of the TLS can be controlled by an external magnetic field. How-

ever, the magnetic-field dependence of the trap spin at low temperatures is suppressed because of the Kondo effect.

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APPENDIX: DERIVATION OF THE EFFECTIVE HAMILTONIAN

In this Appendix we derive an effective low-energy Hamiltonian that corresponds to our model of the trap [Eq. (2)] by integrating out the phonon degree of freedom. This can be done for sufficiently large phonon frequency, such that the phonon always remains in its ground state.

For convenience, we first perform a similarity (“polaronic”) transformation, $\tilde{H} = U^{-1}HU$, where $U = \exp[ip\lambda(\sum_{\sigma} n_{\sigma} - 1)/(m\omega_0^2)]$,

$$\tilde{H} = H_0 + H_T \quad (\text{A1})$$

$$H_0 = \sum_{k\sigma} E_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{\sigma} (E_0 + E_P) d_{\sigma}^{\dagger} d_{\sigma} + (U - 2E_P) n_{\uparrow} n_{\downarrow} + \omega_0 b^{\dagger} b, \quad (\text{A2})$$

$$H_T = T_{cd} \sum_{k\sigma} c_{k\sigma}^{\dagger} d_{\sigma} e^{\tilde{\lambda}(b-b^{\dagger})} + d_{\sigma}^{\dagger} c_{k\sigma} e^{-\tilde{\lambda}(b-b^{\dagger})}. \quad (\text{A3})$$

In the transformed Hamiltonian, the on-site energy and interaction are renormalized, and the electron-phonon interaction now only appears in the tunneling part of the Hamiltonian H_T . Here, we have rewritten the phonon Hamiltonian in the second quantized form, with b^{\dagger} the phonon creation operator, and we introduced a parameter $\tilde{\lambda} = \sqrt{E_P/\omega_0}$.

To find the effective Hamiltonian we utilize the smallness of the tunneling matrix element T_{cd} relative to the other energy scales in the problem. Hence the quantum-mechanical evolution operator $S(+\infty, -\infty) = \exp(-i\int_{-\infty}^{+\infty} dt H)$ can be expanded as

$$S(+\infty, -\infty) = e^{-i\int_{-\infty}^{+\infty} dt H_0} \mathcal{T} e^{\int_{-\infty}^{+\infty} dt \hat{H}_T(t)} \quad (\text{A4})$$

$$= e^{\int_{-\infty}^{+\infty} dt H_0} \left[1 - i \int_{-\infty}^{+\infty} dt \hat{H}_T(t) \right. \quad (\text{A5})$$

$$\left. + \int_{-\infty}^{+\infty} dt \int_{-\infty}^t dt' \hat{H}_T(t) \hat{H}_T(t') + \dots \right], \quad (\text{A6})$$

in terms of the tunneling in the interaction representation, $\hat{H}_T(t) = e^{iH_0 t} H_T e^{-iH_0 t}$.

The electronic part of the evolution operator can be obtained by taking the expectation value over the phonon ground state,

$$S_{\text{eff}} = \langle \Psi_0(x) | S | \Psi_0(x) \rangle. \quad (\text{A7})$$

To perform the phonon averaging, we use the identity

$$e^{\tilde{\lambda}(b^{\dagger}-b)} = e^{-\tilde{\lambda}^2/2} e^{\tilde{\lambda}b^{\dagger}} e^{-\tilde{\lambda}b} = e^{-\tilde{\lambda}^2/2} \sum_{m,n} \frac{(\tilde{\lambda}b^{\dagger})^n (-\tilde{\lambda}b)^m}{n!m!}. \quad (\text{A8})$$

For the linear expansion term [Eq. (A5)] only the $n=m=0$ term of the sum in Eq. (A8) remains. This leads to renormalization of the tunneling matrix element in the effective electronic Hamiltonian by the factor $e^{-\tilde{\lambda}^2/2}$,

$$H_T^{\text{eff}} = \langle \Psi_0(x) | H_T | \Psi_0(x) \rangle = T_{cd} e^{-\tilde{\lambda}^2/2} \sum_{k\sigma} c_{k\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{k\sigma}. \quad (\text{A9})$$

In the second-order terms, Eq. (A6), there is, however, a possibility of virtually creating multiple phonon excitations, with the number of phonons created by $H(t')$ equal to the number of phonons destroyed by $H(t)$. It is easy to see that the terms that do not change the occupancy of the d -level are modified one way, e.g.,

$$\langle \Psi_0(x) | [c_{k\sigma}^{\dagger} d_{\sigma} e^{\tilde{\lambda}(b-b^{\dagger})}]_t [d_{\sigma}^{\dagger} c_{k'\sigma'} e^{-\tilde{\lambda}(b-b^{\dagger})}]_{t'} | \Psi_0(x) \rangle = [c_{k\sigma}^{\dagger} d_{\sigma}]_t [d_{\sigma'}^{\dagger} c_{k'\sigma'}]_{t'} e^{-\tilde{\lambda}^2} \sum_n \frac{\tilde{\lambda}^{2n} e^{in\omega_0(t'-t)}}{n!}, \quad (\text{A10})$$

while the terms that do involve the change in the occupancy (pair tunneling) become, e.g.,

$$[d_{\sigma}^{\dagger} c_{k\sigma}]_t [d_{\sigma'}^{\dagger} c_{k'\sigma'}]_{t'} e^{-\tilde{\lambda}^2} \sum_n \frac{(i\tilde{\lambda})^{2n} e^{in\omega_0(t'-t)}}{n!}. \quad (\text{A11})$$

Clearly, the $n=0$ elements of the sums in Eqs. (A10) and (A11), which correspond to second-order processes *without* creation of virtual phonons, can be interpreted as the second-order terms generated by an expansion of the evolution operator S_{eff} in terms of the effective tunneling Hamiltonian H_T^{eff} . The rest of the sums ($n \neq 0$) in Eqs. (A10) and (A11) form additional contributions to the effective Hamiltonian, H_J and H_{pair} , respectively.

By applying the interaction representation for the operators at time t' , $\mathcal{O}(t') = e^{iH_0(t'-t)} \mathcal{O}(t) e^{-iH_0(t'-t)}$, and integrating over t' , in the single d -level occupancy subspace,

$$H_J = -\frac{J}{2} \sum_{k,k',\sigma,\sigma'} d_{\sigma'}^{\dagger} d_{\sigma} c_{k\sigma}^{\dagger} c_{k'\sigma'} \quad (\text{A12})$$

$$J = T_{cd}^2 e^{-\tilde{\lambda}^2} \sum_{n=1}^{\infty} \frac{\tilde{\lambda}^{2n}}{n!} \left[\frac{1}{E_{k'} - E_0 - E_P + n\omega_0} + \frac{1}{E_0 + U - E_{k'} - E_P + n\omega_0} \right]. \quad (\text{A13})$$

In the single-occupancy subspace, Hamiltonian H_J is equivalent to the standard exchange Hamiltonian $-J\mathbf{S}_d \cdot \boldsymbol{\sigma}_{kk'}$. The first term in the square brackets in Eq. (A13) came from

$[d_{\sigma}^{\dagger}c_{k\sigma}]_l[c_{k'\sigma'}^{\dagger}d_{\sigma'}]_{l'}$, and the second from $[c_{k\sigma}^{\dagger}d_{\sigma}]_l[d_{\sigma'}^{\dagger}c_{k'\sigma'}]_{l'}$. The sum over n can be transformed into an integral,¹² and for the case of the symmetric Anderson model, $E_{k'} - E_0 \approx E_0 + U - E_{k'} \approx U/2$, we find

$$J = 2T_{cd}^2 \int_0^{\infty} dx e^{-(U/2 - E_p)x - \tilde{\lambda}^2 [1 - \exp(-\omega_0 x)]} - \frac{4T_{cd}^2 e^{-\tilde{\lambda}^2}}{U - 2E_p} \quad (\text{A14})$$

This is very similar to the expression obtained in Refs. 11 and 12 for the Holstein-Hubbard model, except for the last

term ($n=0$) that needs to be subtracted out to avoid double counting. In the limit $(U/2 - E_p) \gg \omega_0$ we easily find that $J = 4T_{cd}^2/U$, which is bare exchange-interaction strength, is *not* renormalized by the interaction with the phonons. Nevertheless, the effective hybridization in this regime may be dramatically suppressed according to Eq. (A9). In the opposite limit we find $J=0$.

Similarly the pair tunneling amplitude can be obtained. Finally, the effective evolution operator is

$$S_{\text{eff}} = \exp - i \int_{-\infty}^{+\infty} dt (H_0 + H_T^{\text{eff}} + H_J + H_{\text{pair}}). \quad (\text{A15})$$

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