Renormalization of resonant tunneling in MOSFETs

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We study tunneling between a localized defect state and a conduction band in the presence of strong electron-electron and electron-phonon interactions. We derive the tunneling rate as a function of the position of the defect energy level relative to the Fermi energy of conduction electrons. We argue that our results can explain the large tunneling timescales observed in experiments on random telegraph signals in Si metal-oxide-semiconductor field effect transistors.

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It has been long realized that two-state systems can have profound effects on micro- and nano-scale electronic devices, leading to random switching or apparent low-frequency noise in transport. In the well studied case of Random Telegraph Signals (RTS) in Si Metal-Oxide-Semiconductor Field Effect Transistors (MOSFET), electrostatic measurements reveal that the switching is most likely caused by the fluctuating charge of interface defects [1]. The charge fluctuations on the defects lead to fluctuations in the scattering potential experienced by the carriers. In small devices this leads to bi- or multi-valued fluctuating conductance [1], while in devices with a large number of defects it results in $1/f$-like frequency dependent noise [2].

At low temperatures, the charge fluctuation of the defects are mediated by quantum mechanical electron tunneling between the localized defect states and the itinerant states. The signature of the quantum-mechanical tunneling is the temperature-independent switching rate at low temperatures [3]. In this problem, we must also consider the Coulomb interaction, which in fact makes RTS observable. Tunneling in the presence of strong electron correlations has been of active interest as it exhibits a number of peculiar features. One of these features is the Fermi-edge singularity in the resonant impurity tunneling. The singular dependence of the tunnel rate on the energy of the impurity electron relative to the Fermi energy of conduction electrons was first suggested by Matveev and Larkin [4], whose theory was based on the X-ray emission/adsorption problem. The latter was extensively studied in numerous works, see Ref. [5] and references therein, which have shown that the transition rate is proportional to $E^\alpha$, where $E$ is excess energy relative to the absorption/emission threshold. Nozieres and De Dominicis [6] have demonstrated that the power $\alpha$ is related to the scattering phase shift of the conduction electrons at the core hole potential and it has two essential contributions: a negative one due to exciton-like physics [5], i.e., an attraction between the core hole and excited electron, and a positive one due to the orthogonality catastrophe [7], i.e., an adjustment of the Fermi sea to the appearance of the core hole potential. For a single channel model, i.e., in case of spinless Fermi sea electrons interacting with point-like core hole potential, Nozieres and De Dominicis obtained that

$$\alpha = -(2/\pi)\tan^{-1}(\nu V) + [\tan^{-1}(\nu V)/\pi]^2,$$  \hspace{1cm} (1)

where $\tan^{-1}(\nu V)$ is the scattering phase shift, $\nu$ is the density of states of the conduction electrons and $V$ is the Coulomb interaction strength. In the case of a local defect tunnel-coupled to a conduction channel, the same model applies after making an association between the X-ray electrical field coupling strength $\delta d$ and the tunneling matrix element $\Delta$, and defining the energy $E$ as the difference between the localized level position and the Fermi level. Then, one finds that the tunnel rate between the impurity and the Fermi sea is [4]:

$$\gamma_{\text{in/out}} = \gamma_0 \Theta(\pm E_0) |E_0 \tau_e|^\alpha,$$  \hspace{1cm} (2)

where $\gamma_0 = 2\pi\nu\Delta^2$, $\Theta$ is a step function, $\tau_e$ is the cutoff of the order of the conduction electron Fermi energy and $\alpha$ is given by Eq. (1).

The singular behavior predicted by Eq. (2) has been observed experimentally in the resonant impurity tunneling in Si MOSFETs [3], with a negative exponent $\alpha$. There is, however, a serious discrepancy between the simple theory prediction, Eq. (2), and experiments [3,8] that has to do with the prefactor $\gamma_0$. In particular, in Si MOSFETs the tunneling is found to occur on a rather slow timescale, typically from milliseconds to seconds.

![FIG. 1. (a) Schematics of MOSFETs; (b) Energy diagram for the impurity level and the conducting electrons. Coupling to optical phonons shifts the bare position of the level.](image)

Given such tunneling timescales one might have guessed that the slow tunneling rate is due to a large...
distance, on the order of 15-20 Å, between the impurities and the insulator-semiconductor interface. However, the distance between the resonant impurity and the 2-Dimensional Electron Gas (2DEG) in the MOSFET conducting channel can be determined via a quite simple experimental procedure based on the monitoring of the defect average occupancy as a function of the gate voltage, which reveals that the separations between the impurities and the 2DEG is typically of the order of 1-2 Å [11]. A naive estimate suggests that for such width of the tunnel barrier (of height of several eV) the impurity electron dwell time must be in the range of pico- to nanoseconds, which is by many orders of magnitude smaller than the observed dwell time. In the present work we argue that this apparent contradiction can be resolved if one takes into account strong electron-optical phonon coupling in this local electron-phonon coupling by a Holstein-type Hamiltonian

\[ H_{ph} = g d^d (a^d + a) + \omega_0 a^d a, \]  

where \( a^d(a) \) are creation(annihilation) operators for a local optical phonon of frequency \( \omega_0 \) coupled to the occupation number at the impurity. The coupling constant \( g \) will be estimated later [6].

We now evaluate the defect electron tunneling rate at \( T = 0 \) by calculating the matrix element \( \langle 0| e^{-iT_H} | 0 \rangle \), which is the probability amplitude for the impurity state to remain empty. Here \( H = H_0 + H_{ph} \) and the “ground” state \( |0\rangle \) corresponds to the trap being empty, and the phonon and the conduction electrons in the ground state, i.e., \( |0\rangle = |0\rangle_{el} \otimes |0\rangle_{ph} \otimes |0\rangle_{el} \). We will carry out the calculation in Euclidean time by setting \( it = \beta \). In what follows \( \hbar \) and electron charge \( e \) are set to unity unless stated otherwise.

We expand \( Z = \langle 0| e^{-\beta H} | 0 \rangle \) in terms of the tunneling term in the Hamiltonian \( H \) as

\[ Z = \sum_N \int d^{2N} |\beta \rangle \langle 0| T e^{-\beta H'} T' |\beta_H N \rangle \cdots H_T(\beta_1) |0\rangle, \]  

where we have introduced a shorthand notation \( \int T d^{2N} |\beta \rangle = \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_2} d\beta_1 \), \( T \) is the time ordering operator, and \( N = 0, 1, \ldots \). In Eq. (5) \( H_T(\beta) = \exp (\beta H') H_T \exp (-\beta H') \), where \( H_T = \Delta \sum_k (c^k_+ d^k + d^k c^k) \) and \( H' \) contains all the remaining terms of the Hamiltonian \( H \). Note that \( H' \) is diagonal in \( d^d \) and can be decomposed into two commuting parts, \( H_{el} \) and \( H_{ph} \), that involve conduction electrons and phonons respectively.

The conduction electrons and optical phonons can be integrated out by realizing that a term with given \( N \) in the sum in Eq. (5) corresponds to trap site being occupied for periods of time \( \beta_{2j-1} < \beta < \beta_{2i} \), \( i \leq N \), and being empty otherwise, see Fig. 2(a). One can formally write that term in the sum in Eq. (5) as

\[ e^{-\int_0^\beta H_{el}[n_d(\beta')]d\beta'} |0\rangle_{el} \otimes e^{-\int_0^\beta H_{ph}[n_d(\beta')]d\beta'} |0\rangle_{ph}. \]  

Here the explicitly time dependent Hamiltonians \( H_{el}[n_d(\beta)] \) and \( H_{ph}[n_d(\beta)] \) correspond to the first three terms in Eq. (3) and to Eq. (4) respectively, with the replacement \( d^d \to n_d(\beta) \), where \( n_d(\beta) \) is the occupation number of the trap as a function of time,

\[ n_d(\beta) = \sum_{\beta_{2j-1}}^{\beta} [\Theta(\beta - \beta_{2j-1}) - \Theta(\beta - \beta_{2j})]. \]  

The phonon-dependent matrix in Eq. (6) can be evaluated by a standard method of either cummulant expansion or by path integral techniques as a ground-to-ground
state amplitude of a harmonic oscillator subjected to an external force \( n_d(\beta) \). By using Eq. (7) this matrix element is

\[
e^{-GN}e^{E_p} \sum_j (-1)^j \beta_j \exp [-G \sum_j (-1)^j - k e^{-\omega_0(\beta_j - \beta_k)}], \tag{8}
\]

where we have defined the polaronic shift \( E_p = g^2/\omega_0 \) and \( G = E_p/\omega_0 \). The first exponent in Eq. (8) is due to the diagonal terms \((j = k)\) in the sum over \( j, k \).

The electronic matrix element in Eq. (6), which is essentially the \( N \)-particle propagator for the conduction electrons, can be evaluated in the large \( \beta \) limit by the technique developed by Nozieres and De Dominicis [6], and by Anderson and Yuval [12]. The technique relies on the flat density of states assumption for the Fermi sea electrons (which is the case for the 2DEG in the conduction channel) and is based on the theory of singular integral equations. It allows one to obtain an asymptotically exact expression for the \( N \)-particle Green’s function in Eq. (6) in the limit \( \beta_{2j} - \beta_{2j-1} \gg \tau_e \). By adjusting the result of Refs. [6,12] for the electronic Green’s function in Eq. (6), and substituting Eq. (8) in Eqs. (5,6) we obtain

\[
Z = \sum_N \frac{\gamma_0 e^{-G}}{2\pi \tau_e} N \int d^2N [\beta] e^{-E_R \sum_j (-1)^j \beta_j} \times \exp \left[ j > k \right] \left[ K \ln \left( \frac{\beta_j - \beta_k}{\tau_e} \right) - Ge^{-\omega_0(\beta_j - \beta_k)} \right]. \tag{9}
\]

In Eq. (9) we have defined \( E_R = E_0 - E_p, \gamma_0 = 2\pi \nu \Delta^2 \), and \( K = 1 + \alpha \). Thus, due to the coupling to the phonon mode the resonant level shifts downwards as shown in Fig. 1(b).

To proceed, we write Eq. (9) as the \( T = 1 \) partition function of a one-dimensional ferromagnetic Ising model, where a spin up or down corresponds to an empty or occupied impurity respectively, as shown in Fig. 2(b). The spacing in imaginary time between successive levels equals \( \tau_e \). This Ising model has a nearest neighbor coupling term \((-1/2)\ln(2\pi/\gamma_0 \tau_e) + G s_i s_{i+1} \) \((s_i = \pm 1)\), and a long range interaction \(-1/2 \{ K (i - j)^2 + (G\omega_0^2/\tau_e) \exp(-\omega_0 \tau_e |i - j|) \} s_i s_j \). The renormalized position of the resonant level \( E_R \) plays the role of an external magnetic field. In the weak long-range interaction regime relevant here, \( K < 1 \), the Ising system is in a paramagnetic state composed of ferromagnetic domains whose size is controlled by the short range interaction. A simple estimate for the mean separation between the domain walls at zero external field \((E_R = 0)\) yields \( l \approx \exp(G)/\gamma_0 \gg \tau_e \). The external field \((E_R \neq 0)\) forces spins to align along its direction, thus shrinking the domains opposing the field relative to the ones aligned with the field. The ratio of the corresponding domain sizes can be estimated by evaluating the average magnetization \( \langle s \rangle \) per spin. For \( E_R \gg \gamma_0 \exp(-G/2) \) one gets \( 1 - \langle s \rangle \sim \gamma_0 \exp(-G/(\tau_e E_R^2)) \) and therefore the average size of the domains with spins along the field exceeds that of the domains of spins opposing the field at least by a factor of \( \eta = \tau_e E_R^2/\gamma_0 \exp(-G) \gg 1 \). (The long range terms will favor even more polarized state as they provide additional ferromagnetic coupling.) As a result the interaction between domain walls from different domains is negligible provided \( \omega_0, E_R \gg \gamma_0 \exp(-E_p/\omega_0) \).

The above arguments allow for a significant simplification of the transition matrix element \( Z \) in Eq. (9) in the limit of small \( \gamma_0 \tau_e \exp(-G) \). Retaining only those terms in the last exponent of Eq. (9) that couple \( \beta_{2j} \) and \( \beta_{2j-1} \) we obtain

\[
\sum_N \frac{\gamma_0 e^{-G}}{2\pi \tau_e} N \int d^2N [\beta] \prod_{j=1}^N \phi(\beta_{2j} - \beta_{2j-1}) \tag{10}
\]

where \( \phi(\beta) = \exp[-E_R \beta - K \ln(\beta/\tau_e) + G e^{-\omega_0 \beta}] \). Our approximation is similar to the non-interacting “blip” approximation used in the solution of the spin-boson problem [14] and therefore the same method of Laplace transform can be used to evaluate the sum in Eq. (10). Upon Laplace transform \( \tilde{Z} = \int_0^\infty d\beta e^{-\beta \lambda} \tilde{Z}(\beta) \), which converts the \( N \)-term in the sum into \((\Delta e^{-G})^{2N} (1/\lambda)^N(1/\phi(\lambda))N\), where \( \tilde{\phi}(\lambda) = \int_0^\infty d\beta e^{-\beta \lambda} \phi(\beta) \). Re-summation in Eq. (10) then yields \( \tilde{Z} = (\lambda - \gamma_0/2\tau_e) e^{-G \tilde{\phi}(\lambda)} \). The tunnel rate \( \gamma \) can be associated with twice the imaginary part of the pole of \( \tilde{Z} \). In the limit \( \gamma_0 \tau_e e^{-G} \ll E_R \), the rate \( \gamma \) of tunneling into the impurity is given by

\[
\gamma_0 e^{-G} \int \frac{\gamma_0 e^{-G}}{2\pi \tau_e} \int \exp \left[ -E_R \beta - K \ln(\beta/\tau_e) + G e^{-\omega_0 \beta} \right] d\beta, \tag{11}
\]

In order to evaluate the imaginary part of the above integral an analytical continuation must be used. We follow prescription of Ref. [15]. The procedure is straightforward: at the saddle point \( \beta_0 \) (given by equation \(-E_R - (K/\beta_0) = G \exp(-\omega_0 \beta_0) \)) we deform the contour...
of integration into the complex plane in the direction of steepest descent (along the +i direction in our case). As a result the integral picks up a convergent imaginary part. The numerical result is presented in Fig. 3. In the limiting cases of small and large $E_R$ simple asymptotic expressions for the tunnel rate into the impurity are possible:

$$\gamma_{\text{in}} = \frac{\gamma_0 \Theta(-E_R)}{\Gamma(1 + \alpha)} |E_R \tau_e|^\alpha, \quad |E_R| < \omega_0; \quad (12a)$$

$$\gamma_{\text{in}} = \frac{\gamma_0 \Theta(-E_R)}{\Gamma(1 + \alpha)} [(E_R - E_p) \tau_e]^\alpha, \quad |E_R| > E_p. \quad (12b)$$

In Eqs. (12) $\Theta(z) = (2\pi/z)^{1/2} \times e^{-z}$. For $E_R < E_p$ the rate is suppressed by $\exp(-E_p/\omega_0)$. This suppression occurs in case of elastic tunneling, when no real phonon modes are excited, and essentially represents the overlap of the phonon ground state wave function for occupied and empty defect states. [14]. The exponent $\alpha$ is due the X-ray singularity as in Eq. (2). For $E_R \sim E_p$ the exponential renormalization disappears due to opening of additional inelastic tunneling channels with excited phonons in the final state.

So far we have not included the effects on spin degeneracy. However, based on the close analogy between our results Eqs. (11,12) and the X-ray absorption [6] problem, we argue that the main effect of the spin degeneracy is to change the second term in the expression for the exponent $\alpha$ in Eq. (1) by a factor of 2.

$$\tilde{\Gamma}(0) = (2\pi/\omega)^{1/2} \times e^{-\omega}. \quad \text{For } E_R \ll E_p$$

$$\tilde{\Gamma}(z) = (2\pi/z)^{1/2} \times e^{-z}. \quad \text{For } E_R \sim E_p$$

$$\tilde{\Gamma}(z) = (2\pi/z)^{1/2} \times e^{-z}. \quad \text{For } E_R > E_p$$

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![FIG. 3. Dependence of the tunnel rate on the bias](image)

For the interface impurity states in a Si MOSFET the coupling constant turns out to be sufficiently strong. In order to estimate the order of magnitude of the polaronic shift that enters Eqs. (12) ($E_p = g^2/\omega_0$), we take Fröhlich coupling constants of an electron to an optical phonon mode with a wavevector $k$ [13], $g_k = \alpha(\Psi_d | e^{ikr} | \Psi_d) / (V^{1/2} |k|)$. Here $V$ is crystal volume and $\alpha^2 = 2\pi e^2 \omega_0 (\varepsilon_\infty^{-1} - \varepsilon_0^{-1})$, where $\varepsilon_\infty$ and $\varepsilon_0$ are high frequency and static dielectric constants, $e$ is electron charge and $\Psi_d$ is the wavefunction of the impurity electron. Assuming that the latter is a hydrogen-like ground state with effective Bohr radius $a_d$, one finds that $\langle \Psi_d | e^{ikr} | \Psi_d \rangle = [1 + (a_d k)^2/4]^{-2}$. Using the equivalence between electron-phonon coupling in our single-mode model and Fröhlich’s multi-mode Hamiltonian [10], that is $g^2 = \sum_k g^2_k$, we obtain that $E_p = 5 \varepsilon_0^2 / (16 a_d) (\varepsilon_\infty^{-1} - \varepsilon_0^{-1})$. For a deep impurity level in SiO$_2$, $a_d \sim 1.4$, $\varepsilon_\infty \simeq 2$, $\varepsilon_0 \simeq 4$, we get $E_p \simeq 1$ eV. The frequency of the optical phonons near the SiO$_2$ – Si interface is of the order 60 meV, which yields the renormalization of the tunnel rate in Eq. (12a) by a factor of $\exp(-16) \simeq 10^{-7}$.

While the detailed quantitative theory warrants further study, we believe that our model gives a qualitative explanation for the tunneling slowdown at Si – SiO$_2$ interfaces.

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