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Tunnel-FET Switching Is Governed by Non-Lorentzian Spectral Line Shape

This article provides new insights into fundamental limitations of the tunnel FETs (tFETs) for desirable energy-efficient operations, and how to possibly overcome them.

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ABSTRACT In tunnel field-effect transistors (tFETs), the preferred mechanism for switching occurs by alignment (ON) or misalignment (OFF) of two energy levels or band edges. Unfortunately, energy levels are never perfectly sharp. When a quantum dot interacts with a wire, its energy is broadened. Its actual spectral shape controls the current/voltage response of such transistor switches, from on (aligned) to off (misaligned). The most common model of spectral line shape is the Lorentzian, which falls off as reciprocal energy offset squared. Unfortunately, this is too slow a turnoff, algebraically, to be useful as a transistor switch. Electronic switches generally demand an ON/OFF ratio of at least a million. Steep exponentially falling spectral tails would be needed for rapid off-state switching. This requires a new electronic feature, not previously recognized: narrowband, heavy-effective mass, quantum wire electrical contacts, to the tunneling quantum states. These are a necessity for spectrally sharp switching.

KEYWORDS Field-effect transistors (FETs); quantum dots; resonant tunneling devices

I. EFFECT OF SPECTRAL LINE SHAPE ON TFET SWITCHING

One of the most central problems in physical science is predicting and understanding spectral line shape. A Lorentzian line shape $1/(\Delta \omega^2 + (\Gamma/2)^2)$ is often assumed, where $\Delta \omega$ is the spectral shift from its resonant position and $\Gamma$ is an associated linewidth. However, this form rarely applies in condensed matter physics. In the solid state, the optical spectrum of electronic transitions usually decays exponentially, the so-called Urbach tail $[1]$, $\sim \exp(-\Delta \omega/\Gamma_U)$, with a characteristic Urbach energy $\hbar \Gamma_U$.

This exponential falloff permits materials to be very transparent in the infrared, as required for long-distance optical communication [2] in glass fibers. If the electronic transitions in the glass had a Lorentzian line shape instead, which falls off slowly as $\sim 1/\Delta \omega^2$, the infrared optical absorption would never quite turn off, and the communication attenuation length would be $\sim 1$ m. Lorentzian line shape in glass would be a catastrophe for modern civilization, which relies upon optical fibers for worldwide connectivity.

Despite its importance to telecommunications, there is no physics consensus for a simple, common, origin of...
Urbach tail spectra, though many complex physical models have been proposed [3]–[9].

In this paper, we introduce another instance in which an exponentially decaying spectrum is important in technology, namely, the tunnel field-effect transistor (tFET). tFETs are attractive as an alternative to the MOSFET because they are not fundamentally limited by the thermal subthreshold slope limit of 60 mV/dec [10]. tFETs were first conceived of in the late 1970s [11] and several early theoretical proposals and experimental demonstrations followed in the ensuing couple of decades [12]–[16], although none of them exhibited subthermal subthreshold slopes. In the 2000s and the 2010s, a large variety of device structures and material systems under various thermal, stress, and other physical conditions were investigated [17]–[34], and we now have several theoretical proposals, backed by simulations [35]–[41], and experimental demonstrations [42]–[57] of devices with subthreshold slopes either below 60 mV/dec or very close to it. Unfortunately, the theoretical predictions are not confirmed by the device results. For example, the subthermal subthreshold slope is achieved only for a few decades of current or at very low current levels.

At a fundamental level, the exact shape of the spectral line shape, that is, band tails of materials, plays a crucial role in determining the subthreshold slope of tFETs. This is not widely recognized, though some prior work has been done in this regard [58], [59]. In this paper, we study the problem of spectral line shape in tFETs and deduce criteria that are necessary for a tFET to have exponential subthreshold behavior.

In tFETs, there are two mechanisms as follows, which can be exploited to obtain improvements in the subthreshold slope [60].

1) The tunneling distance can be modulated [61]–[63].
2) The energy levels can be aligned or misaligned between the source and drain, sometimes called the energy-filtering mechanism [64], [65].

Tunnel distance modulation is more common, but its response to control signals becomes less steep and more gradual at precisely the higher conductance densities that are actually needed for driving wires in a circuit [66].

Thus, the preferred mechanism for switching occurs by energy filtering, alignment (ON) or misalignment (OFF), of two energy levels or band edges. Nonetheless, energy levels are never perfectly sharp. Their actual spectral shape controls the current/voltage response of such transistor switches, from on (aligned) to off (misaligned).

The ON-state is illustrated in Fig. 1(a) in which a valence band quantum well faces a conduction band quantum well. Tunneling occurs from the highest valence band level to the lowest conduction band level, as illustrated by the green arrow. External electrical contact, to the quantum wells, is illustrated by the resistors R connected to the quantum levels in Fig. 1(a). These are usually tunnel resistors. Off-switching occurs when the two quantum levels are misaligned, as shown in Fig. 1(b). Since the quantum levels have finite linewidth, the switching process is actually gradual, depending on level sharpness. In Fig. 1(b), tunneling occurs over a range of energies, a convolution between the spectral density on one side and the spectral density on the other side. Tunneling between the two spectral tails is illustrated by the red arrow. If the spectral sharpness is insufficient, the current does not turn off.

The most commonly assumed model of spectral line shape is the Lorentzian

\[ S(\Delta \omega) \sim 1/(\Delta \omega^2 + (\Gamma/2)^2), \]

which is associated with the familiar time-domain exponential decay of population \(\sim \exp(-\Gamma t)\). However, away from the line center, Lorentzian line shape falls off as \( S(\Delta \omega) \sim 1/\Delta \omega^2 \), which is algebraically too slow to function as a transistor switch. Switches generally demand at least \(10^6\) ON/OFF ratio. Sharper spectral tails are needed.

Fortunately, experimental observations in condensed matter show that the broad spectral tails associated with the Lorentzian line shape are the exception rather than the rule. Line shapes with exponentially falling spectral tails are a necessity for the energy-filtering mechanism in tFETs. In this paper, we will derive the origin of rapidly falling exponential spectral wings

\[ S(\Delta \omega) \sim \exp(-\Delta \omega/\omega_0) = \exp(-2\Delta \omega \tau_p) \]

where \(\omega_0 = 1/2\tau_p\) is a desired decay constant in the frequency domain. This spectral shape provides the required rapid turnoff mechanism for tFET electrical switches.

Exponential spectral tails can occur in tunneling but may also apply to other spectral line shape phenomena in physics and chemistry. Indeed, exponentially falling spectra are common in condensed matter, but broad Lorentzian spectra are rare.

\[1\)In the above, band tails means well beyond the central full-width at half-maximum (\(\Delta \omega \gg \text{FWHM}\)).
II. LIFETIME BROADENING OF QUANTUM DOT TO A WIRE CONTACT

We envision the tunnel switch to be nanoscopic, consistent with Moore’s law. Thus, there is no loss of generality by considering the lowest energy state of the conduction band shown in Fig. 1 to be an isolated quantum level or dot, and likewise for the highest valence band level acting as a single quantum dot. Our goal is to assign a spectral shape to the individual dots. An empty conduction band quantum dot will accept an electron by tunneling. However, the dot is connected to a wire contact and the electron will leak away, increasing the spectral linewidth by lifetime broadening.

The spectrum \( S(\Delta \omega) \) associated with electrical contact to the quantum dot is the Fourier transform of the amplitude decay represented by the projection \( \langle \Psi(0) | \Psi(t) \rangle \), of the decayed quantum dot state \( |\Psi(t)\rangle \), onto the original filled quantum dot wave function \( |\Psi(0)\rangle \). Since we are considering only simple\(^2\) lifetime broadening of the quantum dot, the amplitude as represented by \( \langle \Psi(0) | \Psi(t) \rangle \) is positive and decaying to zero. The spectral broadening is the Fourier transform of the wave function correlation function \( S(\omega) = \int_{-\infty}^{\infty} \langle \Psi(0) | \Psi(t) \rangle e^{-i\omega t} dt \), which simplifies into the cosine transform given by \( S(\omega) = 2\int_{0}^{\infty} |\langle \Psi(0) | \Psi(t) \rangle|\cos(\omega t)dt \).

Thus, there is a simple Fourier link between the amplitude decay and spectral shape, as illustrated in Fig. 2. For example, the Lorentzian spectral line shape \( 1/(\Delta \omega^2 + (\Gamma/2)^2) \), the red curve in Fig. 2(b), when subject to an inverse Fourier transform back to the time domain, becomes the classic exponential time decay \( \exp(-t/\tau) \), as illustrated by the blue curve in Fig. 2(a). Conversely, exponential tails in the frequency domain result from an initial quadratic (nonexponential) decay in the time domain, as we show now.

In fact, every good quantum mechanics textbook \([69]\) warns that for early times, the quantum amplitude actually falls quadratically \( 1 - t^2/8\tau_p \), far more slowly than the initial linear decay expected from \( \exp(-t/2\tau) \), as illustrated by the blue curve in Fig. 2(a). This slow initial quadratic decay in time eventually reverts to the familiar exponential time decay, after a brief induction period \( 2\tau_p \).

The shape of the early time decay \( t/\tau \ll 1 \) controls the spectrum at a high spectral shift \( \Delta \omega \gg \text{FWHM} \). Early time quadratic decay when transformed back to the frequency domain leads to exponential spectral tails \( S(\Delta \omega) \sim \exp(-2\Delta \omega \tau_p) \) [the blue curve in Fig. 2(b)] rather than broad Lorentzian spectral tails [the red curve in Fig. 2(b)]. Initial quadratic decay is sufficient to produce exponential tails that provide strong OFF-state switching in tFETs.

To put it succinctly, in our model, lifetime broadening is controlled by two times, \( \tau \) and \( \tau_p \), where \( \tau_p \leq \tau \).

\(^2\) Phase-dependent broadening associated with complex amplitude decay and T\(_2\)-type broadening will further challenge tFET performance.
Fig. 3. (a) Conventional picture of lifetime broadening due to decay from the quantum dot level |Ψ⟩ to a contact continuum, using Fermi’s golden rule. (b) Inserting a narrowband wire between the quantum dot and the contact will ensure that the initial decay of the electron population of the quantum dot is quadratic, leading to exponential line shapes.

\[ \Gamma \equiv 1/\tau = (2\pi/h)|X|^2(dN/dE), \] as illustrated in Fig. 3(a).

This implies the exponential decay of quantum dot amplitude \(|\langle \Psi(0)\rangle |\Psi(t)\rangle|\sim\exp(-t/2\tau).\) The corresponding Lorentzian line shape \(1/(\Delta\omega^2 + (1/2\tau)^2)\) is incompatible with the required TET ON/OFF ratio. Implicit in Fermi’s golden rule is that the tunneling matrix element \(X\) couples to an infinite range of energy states in the wire, \(dN/dE\). In this case, the exponential \(\exp(-t/2\tau)\) begins right at \(t = 0\), and we are stuck in the Lorentzian behavior (the red curves in Fig. 2).

By contrast, the blue curves in Fig. 2(b), which contain exponential tails in the frequency domain, can be obtained by truncating to a narrower density of final states \(dN/dE\) with a finite bandwidth \(E_{narrow-bandwidth}\) spread over \(\pm h/2\tau_p\), as shown in Fig. 3(b). This achieves the initial parabolic decay for a time \(2\tau_p\), as indicated in Fig. 2(a). Thus, we would benefit from a mechanism that limits the bandwidth of the density of final states. We must isolate the final state from the wire so that it does not broaden much. At the same time, the current flow must not be restricted. One way of doing this is to introduce a narrowband wire, with a small electron energy bandwidth, between the quantum dot and the actual metal contact, as shown in Fig. 3(b). Having a narrowband final density of states to tunnel into, as opposed to a large bandwidth final density of states, ensures that the decay of electron population in the quantum dot is quadratic for short times. This early time quadratic behavior translates into exponential tails in the energy domain. Despite the heavy effective mass, the narrowband wire, there is no loss in conductivity, which is controlled by the conductance quantum in the ballistic regime.

The narrowband wire that receives electrons from the quantum dot itself has a finite density of states, \(dN/dE\), with bandwidth \(h/\tau_p\). Then, an initial parabolic amplitude-induction period \(2\tau_p\) for the initial \(|\Psi(t)\rangle\) quantum dot decay is guaranteed. This is later followed by the normal exponential quantum dot decay by Fermi’s golden rule, \(|\langle \Psi(0)\rangle |\Psi(t)\rangle|\sim\exp(-t/2\tau),\) as shown by the blue curve in Fig. 2(a), \(\tau_p \leq \tau\).

The initial parabolic decay can be explained as follows. The amplitude decay of an electron from the quantum dot in two sequential steps: initially, there is a coherent evolution between the quantum dot state \(|\Psi\rangle\) and the state at the tip of the narrowband wire. These oscillate at an angular frequency \(2|X|/\hbar\). This manifests itself initially as a quadratic decay of quantum dot amplitude

\[ |\langle \Psi(0)\rangle |\Psi(t)\rangle| = \sqrt{1 - (|X|t/\hbar)^2} = 1 - |X|^2t^2/2\hbar^2.\]

This initial oscillation is terminated at time \(t = 2\tau_p\) by the exponential time decay \(\tau\), long before even one oscillation is completed, \(\tau_p \ll \hbar/|X|\).

The resulting time decay of the quantum dot amplitude is plotted in blue in Fig. 2(a), with the corresponding lifetime broadened spectrum in blue in Fig. 2(b), for the specific case of \(\tau_p = 0.1\tau\).

The value of \(1/\tau\) can be calculated by plugging in the value of the final density of states into Fermi’s golden rule. The final state is now the tip state of the narrowband wire for which the peak value of the density of states is \(dN/dE = 2\tau_p/\pi\hbar\). Hence, the later, exponential portion of the \(|\langle \Psi(0)\rangle |\Psi(t)\rangle|\rangle\) decays as

\[ 1/\tau = (2\pi/h)|X|^2(dN/dE) = (2\pi/h)|X|^2(2\tau_p/\hbar). \quad (1) \]

In summary, the electron population in the quantum dot experiences an initial quadratic decay given by

\[ \rho_{dot}(t) = 1 - (|X|t/\hbar)^2 \quad (2) \]

for a period of \(2\tau_p\) followed by an exponential decay given by

\[ \rho_{dot}(t) = \exp(-t/\tau) = \exp(-2\pi/h)|X|^2(2\tau_p/\pi\hbar)t. \quad (3) \]

The short-time and long-time behaviors above can be stitched together using the following fitting function:

\[ \rho_{dot}(t) \sim \exp(b - \sqrt{b^2 + (t/\tau)^2}) \quad (4) \]

where \(b = h^2/2(|X|^2\tau)^2 = 2\tau_p/\tau\). This function has the correct limits at short and long times and expands in even powers of time only, starting out quadratically at \(t = 0\). The blue curves, plotted in Fig. 2, comprise this approximate temporal form \(\rho_{dot}(t) \sim \exp(b - (b^2 + (t/\tau)^2)^{1/2})\), in Fig. 2(a), and its Cosine transform spectrum, in Fig. 2(b). The initial temporal quadratic decay of occupation probability guarantees exponentially falling spectral tails, the main topic of this paper.
As an aside, the physics of a quantum dot coupled to a narrowband wire is analogous to an atom weakly coupled to an electromagnetic cavity with a cavity decay time $\tau_p$. If $\tau_p \ll \hbar/|X|$, the cavity is very lossy, and we call this weak coupling; if $\tau_p \gg \hbar/|X|$, a very high-Q cavity, we call it strong coupling. In the optical case, $|X|$ would be the Rabi matrix element between the excited atom and the electromagnetic cavity. The corresponding weak coupling optical cavity is shown in Fig. 4. The analogy is incomplete, given that in the open optical cavity, the excited atom could directly decay by vertical spontaneous emission, an alternative to cavity loss. The correspondence is reestablished if that external emission is regarded as a weak probe. This suggests that the lifetime broadening of an excited atom, in weak coupling with an electromagnetic cavity, has an exponentially decaying spectral line shape, rather than Lorentzian, which is worth testing.

IV. CURRENT–VOLTAGE CHARACTERISTICS OF THE ENERGY FILTERED tFET

Neglecting the very brief initial quadratic period $\tau_p$, there is a finite mean lifetime $\tau$ for an electron to remain on the dot or conversely to jump back to the dot from the narrowband wire. If the quantum dot is occupied, but the narrowband wire states are unoccupied, the maximum current flow is $\sim 2q/\tau$, where the value 2 arises from two possible spin states. If there is a Fermi–Dirac distribution with occupation $f_d$ and Fermi level $E_{Fd}$ on the dot, and corresponding $f_w$ and $E_{Fw}$ on the narrowband wire, the net current is diminished as $(2q/\tau)(f_d - f_w)$, upon allowing for reverse current. For Fermi–Dirac statistics, the difference in occupation is $(f_d - f_w) \sim (E_{Fd} - E_{Fw})/4kT$, as given in [71]. Therefore, the current flow $I = (2q/\tau)(q\Delta V/4kT)$ is proportional to voltage difference, and we can define a conductance of the tunnel contact to be $G_{contact} \equiv (2q/\tau)(q/4kT)$ in the low-voltage regime $\Delta V < 4kT$. By taking account of thermal occupation in this way, a tunneling current can be converted to a conductance. (Using the uncertainty principle inequality, $\hbar/\tau \leq q\Delta V$, $G_{contact}$ is always $\leq q^2/\hbar$, the quantum of conductance, for a single tunneling channel.)

The tFET is built from two quantum dots, as shown in Fig. 5(a), which is a graphene nanoribbon example. As electrons transition from a filled valence band dot to an empty conduction band dot, we can calculate the current and then convert it to conductance. When the energy levels are aligned, the dot–dot peak current can be written by

\[ h = \frac{q^2}{\hbar} \]

\[ \text{volts per decade} \]

\[ \text{millivolts per decade} \]

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Lorentzian quantum dots. The Lorentzian spectrum has unacceptable leakage. For this numerical example, \( dN/dE \) 

\[
I_0 = 2q \frac{2\pi}{h} |M|^2 \frac{\tau}{\pi h}
\]

where \( M \) is the Hamiltonian matrix element between the two quantum dots, \( dN/dE_c \) is the density of states of the empty conduction band dot \( c \), and \( h/\tau \) is its energy FWHM associated with the lifetime broadening of the conduction band quantum dot \( c \). There is an extra prefactor 2 to account for tunneling of both electron spins. For \( dN/dE \), it is safe to use a normalized Lorentzian line shape: 

\[
dN/dE_c = \frac{(2\pi/\tau)h}{(1 + 4\omega^2\tau^2)}
\]

since the current normalization hardly depends on the band tails at all. In this case, the valence band dot is sharp but the conduction band dot is broadened.

Consider that the current at the first conductance band energy level is also broadened, the current equation needs to be modified by averaging over the distribution \( dN/dE_v \). The dot–dot peak current when the two density-of-states distributions are aligned is

\[
I_{\text{peak}} = 2q \frac{2\pi}{h} |M|^2 \int_{-\infty}^{\infty} \frac{dN}{dE_c} |M|^2 \frac{\tau}{\pi h}
\]

where \( T = 0 \) K indicates a completely filled valence band dot and a completely empty conduction band dot. Because of the gate-induced offset between \( E_c \) and \( E_v \), it could be that the region of common overlap will only occur in the band tails. Then, all the considerations of spectral tail shape will control the turnoff current characteristics. The predicted current–voltage curve for offset levels is shown in Fig. 6. The red curve shows the current–voltage behavior when the line shape is Lorentzian, while the blue curve is for the case of exponential line shapes. The current is normalized to \( I_0 = 2q(2\pi/h)|M|^2/\tau \). 

\[
I_{0K} = 2q \frac{2\pi}{h} |M|^2 \int_{-\infty}^{\infty} \frac{dN(E-E_c)}{dE} \frac{dN(E-E_v)}{dE} |M|^2 \frac{\tau}{\pi h}
\]

\[(7)\]

where \( \Delta = (E_c - E_v)/q \).

If operating at \( E_c - E_v < 4kT \), there will be partial occupation of both quantum dots and the current will be: 

\[
\Delta I = I_{0K}(q\Delta V/4kT),
\]

leading to a conductance \( G \equiv I_0/(q/4kT) \).

As long as the spectral tails are exponential, \( S(\Delta\omega) \sim \exp(-2\omega\tau_p) \), converting from frequency to voltage, and fall off as \( dN/dE \) \( \sim \exp(-2\Delta\omega V/\tau_p) \) \( \sim \exp(-\Delta V/V_o) \), the conductance tail will also fall exponentially, with the voltage swing \( \equiv 2.303V_o \equiv (2.303h/(2q\tau_p)) = 6 \text{ mV/decade} \) for the value of \( \tau_p \) specified in the caption of Fig. 6.

V. ON-STATE CONDUCTANCE LIMIT

In [72] and [73], it was shown that the matrix element \( |M| \) coupling the two quantum dots cannot be made arbitrarily large. \( |M| \) must be smaller than the damping linewidth, \( |M| < h/4\tau \). If \( |M| \) were any larger, strong coupling between the two dots would occur. Under strong coupling, the electron would oscillate back and forth between quantum dots, and Lorentzian line shapes could return, making it impossible to turn the device off. Inserting \( |M| = h/4\tau \) into Fermi’s golden rule, the maximum tunneling current from (6) becomes \( \sim q/4\tau \), which leads to tFET conductance, \( G_{\text{FET}} \equiv (q/4\tau)(q/4kT) \). Unfortunately, this is four times less than \( G_{\text{contact}} \).

In effect, the operating tFET consists of three resistors in series, the two contact resistors on either side and the central tunnel resistor that is at least four times larger resistance. At best, the conductance of the device would be one-sixth of the contact conductance, which is itself limited by the quantum of conductance \( 2e^2/h \). To drive the wire capacitance rapidly enough, many such quantum dot tFETs would be required to operate in parallel.
Agarwal and Yablonovitch [72], [73] also provide a useful estimate of the tunneling matrix element $|\mathbf{M}| = E_z \sqrt{\text{Tr}}$, where $E_z$ is the kinetic energy of ground state of the quantum dot, and Tr is the tunneling transmission probability. This formula can connect transmission probability to meaningful currents and voltages from Fermi’s golden rule, recognizing that Tr is always $<1$. The mathematical relationships among dot lifetime $\tau$, tunnel transmission probability $\text{Tr}$, quantum confinement energy $E_z$, currents, and conductances are summarized in Table 1.

### Table 1 Summary of Formulas Connecting the TFET Electrical Properties With the Quantum Mechanical Parameters of the Device.

<table>
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<th>Quantities</th>
<th>Formula</th>
</tr>
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<tbody>
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<td>(a) Single-channel wire–wire conductance vs. transmission probability</td>
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<td>(i) Dot-dot matrix element versus dot-dot transmission probability</td>
<td>$</td>
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<td>(j) Dot-dot current at $T=0K$ versus the convolved density of states</td>
<td>$I_{0K} = 2q \frac{2\pi}{\hbar}</td>
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<tr>
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<tr>
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<td><img src="image-url" alt="Diagram" /></td>
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VI. CONCLUSION

To achieve a very steep slope in tFET response, many requirements must be fulfilled. Gate efficiency must be good. Defect-level concentration producing parasitic leakage must be very low. In addition, the energy levels must themselves be very sharp. The usual assumption
of Lorentzian spectral broadening would not provide sufficient ON/Off ratio to satisfy system needs. A correct use of Fermi’s golden rule provides a mechanism for exponentially falling tunneling spikes, as required for a steep response. This demands that a narrowband, heavy effective mass, wire should mediate between the tunneling energy levels and the external metallic contacts. There are many additional requirements, including the need for the tunneling matrix element $|\mathbf{M}|$ to be reduced such that the system does not enter strong coupling but large enough to provide the maximum conductance.

In this paper, we have shown that exponential spectral tails can arise naturally as part of lifetime broadening, from the initial parabolic decay of population as provided by the more complete form of Fermi’s golden rule given here. In turn, exponential spectral tails justify the concept of exponential steepness or voltage swing, as had always been assumed in TFETs.

In this paper, we have only considered $T_1$ or population decay processes. There may be many other contributions to spectral broadening including $T_2$ processes which will provide further challenge tFET performance.


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Dr. Yablonovitch has been elected to the NAE, NAS, NAI, AmAcArS, and as a Foreign Member, U.K. Royal Society. He was a recipient of the OSA Ives/Quinn Medal, the Benjamin Franklin Medal, the IEEE Edison Medal, the Buckley Prize of the American Physical Society, and the Isaac Newton Medal of the U.K. Institute of Physics.