Insights into electron transport in a ferroelectric tunnel junction

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Abstract

The success of a ferroelectric tunnel junction (FTJ) depends on the asymmetry of electron tunneling as given by the tunneling electroresistance (TER) effect. This characteristic is mainly assessed considering three transport mechanisms: direct tunneling, thermionic emission, and Fowler-Nordheim tunneling. Here, by analyzing the effect of temperature on TER, we show that taking into account only these mechanisms may not be enough in order to fully characterize the performance of FTJ devices. We approach the electron tunneling in FTJ with the non-equilibrium Green function (NEGF) method, which is able to overcome the limitations affecting the three mechanisms mentioned above. We bring evidence that the performance of FTJs is also affected by temperature, in a non-trivial way, via resonance (Gamow-Siegert) states, which are present in the electron transmission probability and are usually situated above the barrier. Although the NEGF technique does not provide direct access to the wavefunctions, we show that, for single-band transport, one can find the wavefunction at any given energy and in particular at resonant energies in the system.

Keywords: ferroelectric tunnel junction; electron transport; non-equilibrium Green function; resonance states; empirical tight-binding

I. INTRODUCTION

The asymmetric ferroelectric tunnel junction (FTJ), a thin ferroelectric (FE) film sandwiched between two dissimilar metallic electrodes or with different interfaces in the case of the same electrode material(Fig. 1), is a promising electron device for many applications such as low power memories [1] or neuromorphic computing [2]. The salient mechanism of FTJ is based on the tunneling electroresistance (TER) effect, i. e., a change in the electrical resistivity when the electric polarization is reversed under external electric field [3, 4]. In other words, the electrical resistance of FTJ switches from a high conduction (ON) state to the low conduction (OFF) state or vice-versa when a high voltage pulse is applied. Ferroelectrics like BaTiO₃, PbZr₀.₂Ti₀.₈O₃, BiFeO₃ [5-7] as well as high-k dielectrics like HfO₂, Hf₀.₅Zr₀.₅O₂ [8, 9] have been shown to work as FTJs. The latter are particularly attractive since they a compatible with CMOS technology.

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The TER effect that is based modulation of the barrier potential upon the polarization reversing can be characterized the TER ratio

\[ \text{TER} = \frac{(J_{ON} - J_{OFF})}{J_{ON}}, \]

where \(J_{ON/Off}\) are current densities in the two different states. The higher the TER ratio and the \(J_{ON}\), the better is the FTJ performance. The extent of barrier modulation depends on numerous factors, such as: i) the thickness and spontaneous polarization of the ferroelectric film, ii) the bias voltage, iii) the difference between work functions and also between screening lengths of electrodes, iv) the built-in field and screening of the polarization charge, as well as the variation of barrier thickness due to piezoelectricity [10].

To understand, describe, and model the TER effect, the \textit{ab-initio} methods may provide an accurate image of the physics governing FTJ systems like the geometry, polarization, electronic structure [11], and transport properties [12 13]. Nevertheless, \textit{ab-initio} methods require large computational resources, which may prevent their intensive use in the early stages of FTJ design, when there is a requirement of a quite fast scan in parameter space to obtain a device with required functionalities. In the search of optimized devices, the semi-empirical methods are fast and, despite all simplifications, are extremely useful for the treatment of the charge transport as long as they are fed with appropriate physical parameters [14 15]. These semi-empirical methods are based on the non-equilibrium Green function (NEGF) method that can calculate exactly, in principles, the tunneling current and the I-V characteristic in an FTJ [15].

In semi-empirical methods based on NEGF the parameters can be adjusted to match the experimental data [14]. In many cases, in order to characterize the electron transport in FTJs and interpret the I-V curves, various models of transport mechanisms involving direct tunneling, thermionic emission, and Fowler-Nordheim tunneling are used [16]. Direct tunneling presumes low energy for incident electrons such that tunneling probability doesn’t depend on the profile of the barrier, which is assumed to be rectangular on average in the case of Simmons formula [17 18] or trapezoidal in the case of Brinkman et al. formula [18 19]. Thermionic emission is that part of the current carried over the top of the barrier by thermally activated charge carriers [20]. The last mechanism, the Fowler-Nordheim tunneling, is used for triangular barrier profiles which are encountered at finite applied bias voltages [21]. The treatment of the above mechanisms is based on some approximations for
electron transport. Simmons and Brinkman et al. as well as the Fowler-Nordheim formulae are based on the semi-classical WKB approximation \cite{17, 21}, while thermionic emission tacitly assumes a homogeneous transmission probability of one for all electrons with energy above the top of the barrier \cite{20}.

FIG. 1. Schematic representation of an FTJ: a ferroelectric (FE) barrier between two metallic electrodes (ML and MR). The dotted line delimitate the electronic device that is considered for calculation.

In this work, by the exact treatment of the tunneling within the NEGF method, we show that the above models describing direct tunneling, thermionic emission, and Fowler-Nordheim tunneling are not accurate enough for performance characterization of the FTJs. These models cannot capture resonant features emerging in FTJ structures that might play an important role in carrier transport and ultimately in the performances of device. The electric current of an impinging electron at a given energy is determined by the electron transmission probability at that energy weighted (multiplied) by its Fermi-Dirac distribution function. Hence, even though they seem unlikely to play a role in the tunneling due to relative simple structure of the barriers, the resonances can contribute significantly to the electric current since their contribution to transmission probability may offset temperature-dependent Fermi-Dirac factor. In the following we will show that the resonances emerging close or above the top of the barriers play a decisive role for transport at room temperature,
fact that is not captured by the simple models previously mentioned. Moreover, resonances may appear in composite (both a ferroelectric and a dielectric) barriers. The NEGF method can accurately describe also these types of heterostructures. Generally, the NEGF approach cannot provide full access to the wavefunctions especially for multi-band transport \[22\], however for a single-band transport we show that this is not the case, the eigenvectors of the spectral functions are just the wavefunctions of the system. At this stage we are able to identify the Green function of the device as the discrete version of the outgoing Green function which is used in diverse scattering problems like nuclear reactions \[23\] or electron transport in nanostructures \[23\] \[24\]. The advantage of such correspondence is that the NEGF of the device and the transmission probability can be expanded as a sum of resonance or Gamow-Siegert states \[23\] \[26\]. Thus we are able to sort out the resonances that count for the electron transport in FTJs.

The paper is organized as follows. The next section deals with the theoretical background: the calculation of polarization induced electrostatic potential across the FTJ, the calculation of transport quantities like I-V curve and conductance by NEGF method, and the evaluation of wavefunctions and resonance states from NEGF calculations. The third section presents numerical results regarding the effect of temperature on electric conductance and TER ratio for several practical cases of simple or composite BaTiO$_3$ based FTJs. In addition, the wavefunctions and resonance states for such FTJ structures are analyzed. The fourth section summarizes the conclusions of this work. Lastly, in the Appendix we present the steps to obtain a discrete tight-binding Hamiltonian from the BenDaniel and Duke Hamiltonian \[22\].

II. THEORETICAL BACKGROUND

A. The profile of potential barrier

In semi-empirical methods the calculation of tunneling current and electric conductance is performed by solving simultaneously the electrostatic and transport problems. They are intricately interrelated since the charge density in Poisson equation is calculated self-consistently from the NEGFs \[22\]. However, when one deals with free carriers only in the metallic contacts they can decouple each other. So, let us first deal with the electrostatics and the profile of the barrier potential. In the following we treat the composite FTJ, where the barrier is
composed of a dielectric and a ferroelectric layer. If the thickness of dielectric is fixed to \( t_{DE} \) and that of the ferroelectric to \( t_{FE} \), we assume that the dielectric and ferroelectric are located for \( x \) between \(-d_{FE}\) and 0 and for \( x \) between 0 and \( t_{FE} \), respectively, while the metallic contact ML is at \( x < -d_{FE} \) and the metallic contact MR is at \( x > t_{FE} \). A widely used and good approximation of the electrostatics in metals is the Thomas-Fermi approximation \[14, 27\]. Within this framework, the electrical fields in ML and MR are given by

\[
E_{ML}(x) = \tau_S e^{(x+t_{DE})/\lambda_1}/(\varepsilon_1\varepsilon_0),
\]

\[
E_{MR}(x) = \tau_S e^{-(x-t_{FE})/\lambda_2}/(\varepsilon_2\varepsilon_0).
\]

In Eqs (2) and (3) \( \tau_S \) is the screening charge at ML/dielectric and ferroelectric/MR interfaces, \( \lambda_1(\varepsilon_1) \) and \( \lambda_2(\varepsilon_2) \) are the Thomas-Fermi screening lengths (dielectric constants) of ML and MR, respectively, and \( \varepsilon_0 \) is the vacuum permittivity. In the following we respectively denote by \( \varepsilon_{FE}, E_{FE}, \) and \( P \) the dielectric constant, the electric field, and the intrinsic polarization of ferroelectric and by \( E_{DE}, \varepsilon_{DE} \) the electric field and the dielectric constant of the dielectric. The electrostatic equations are in fact the continuity of the normal component of the electric induction \( \mathbf{D} \) at both ferroelectric/MR and ML/dielectric interfaces

\[
\tau_S = \varepsilon_{FE}\varepsilon_0 E_{FE} + P = \varepsilon_{DE}\varepsilon_0 E_{DE}.
\]

Additionally, the bias voltage across the structure obeys the equation

\[
\frac{\tau_S \lambda_1}{\varepsilon_1 \varepsilon_0} + \frac{\tau_S \lambda_2}{\varepsilon_2 \varepsilon_0} + E_{FE} t_{FE} + E_{DE} t_{DE} + V + V_{BI} = 0
\]

where \( V \) is the applied voltage and \( V_{BI} \) is the built-in voltage bias due to mismatch of the conduction bands (conduction band discontinuities) and of Fermi energies \( E_{FL} (E_{FR}) \) of ML(MR)

\[
V_{BI} = (\phi_2 + \phi_C - E_{FR} - \phi_1 + E_{FL})/e.
\]

In Eq. (6) \( e \) is the elementary electric charge, \( \phi_1 \) is the band discontinuity at the first interface between ML and the dielectric, \( \phi_2 \) is the band discontinuity at the second interface between the ferroelectric and MR, and \( \phi_C \) is the band discontinuity at the interface between
the dielectric and ferroelectric when the ferroelectric is unpolarized. Eliminating $E_{FE}$ and $E_{DE}$ from Eqs. (4) and (5) we obtain the screening charge $\tau_S$

$$\tau_S = \frac{V + V_B + t_{DF}P/\varepsilon_{0}\varepsilon_{FE}}{\lambda_1 \varepsilon_{0}\varepsilon_{1} + \lambda_2 \varepsilon_{0}\varepsilon_{2} + \frac{t_{DF}}{\varepsilon_{0}\varepsilon_{FE}} + \frac{t_{DE}}{\varepsilon_{0}\varepsilon_{DE}}}.$$  

(7)

Now it is straightforward to obtain the electric potential and the barrier profile knowing that the electric field is homogeneous in both the dielectric and the ferroelectric

$$U (x) = \begin{cases} 
-e\frac{\tau_s}{\varepsilon_{1}\varepsilon_{0}} \exp \left[ \frac{x}{\lambda_1} \right], & x < -t_{DE} \\
-e\tau_s \left( \frac{\lambda_1}{\varepsilon_{1}\varepsilon_{0}} + \frac{t_{DE}}{\varepsilon_{DE}\varepsilon_{0}} + \frac{x}{\varepsilon_{DE}\varepsilon_{0}} \right) - \varphi_1, & -t_{DE} \leq x < 0 \\
-e\tau_s \left( \frac{\lambda_1}{\varepsilon_{1}\varepsilon_{0}} + \frac{t_{DE}}{\varepsilon_{DE}\varepsilon_{0}} \right) - e\frac{\tau_s}{\varepsilon_{FE}\varepsilon_{0}} x - \varphi_1 + \varphi_C, & 0 \leq x \leq t_{FE} \\
e \left( V + V_B + \frac{\tau_s}{\varepsilon_{1}\varepsilon_{0}} \exp \left[ -(x-t_{FE})/\lambda_2 \right] \right) - \varphi_1 + \varphi_C + \varphi_2, & x > t_{FE}
\end{cases}$$

(8)

In Eq. (8) $P$ is considered positive when points from ML to MR and negative when it points the other way around.

**B. Transport by NEGF**

Transport properties like electric current density and conductance can be calculated by solving the Schrödinger equation with scattering boundary conditions, i.e., either an incoming wave from the left or from the right. For a single band, the equation is merely 1D with a BenDaniel and Duke Hamiltonian, where the effective mass of electrons can vary across the structure [22]:

$$H = -\frac{\hbar^2}{2} \frac{d}{dx} \left( \frac{1}{m^* (x)} \frac{d}{dx} \right) + \frac{\hbar^2 k^2}{2m^* (x)} + U (x).$$

(9)

In Eq. (9) it is assumed that the energy band is parabolic with an isotropic effective mass in each layer of the nanostructure, $k$ is the transverse wavevector (parallel to each interface), $m^*$ is the effective mass, and $U(x)$ potential energy given by Eq. (8). Equation (9) can be discretized into 1D problem in a tight-binding representation [22]. The details are presented in the Appendix. The Hamiltonian in the matrix format has the following tridiagonal form
\[
H = \begin{pmatrix}
H_L & V_{LD} & 0 \\
V_{LD}^\dagger & H_D & V_{RD}^\dagger \\
0 & V_{RD} & H_R
\end{pmatrix}.
\] (10)

In this format one can easily see that the Hamiltonian has three parts: the semi-infinite left (L) and right (R) metallic electrodes and the device (D) that is defined by \(H_D\), an \(n_D \times n_D\) matrix. Both electrodes act as reservoirs, hence they have well defined chemical potentials and temperatures. We can define the retarded Green function \(G^R\) of the system at energy \(E\) as the inverse matrix of \([(E + i\eta) - H]\), where \(\eta = 0^+\). Similarly the advanced Green function \(G^A\) is the inverse of \([(E - i\eta) - H]\), i. e.,

\[
G^{R,A}(E) = [(E \pm i\eta) - H]^{-1}.
\] (11)

In the NEGF method one eliminates the degrees of freedom of contacts by introducing self-energies into the projected Green functions of the device (D)

\[
G^{R,A}_D(E) = \left[(E \pm i\eta) - H_D - \Sigma^{R,A}_B(E)\right]^{-1}.
\] (12)

The self-energy \(\Sigma^{R,A}_B(E) = \Sigma^{R,A}_L(E) + \Sigma^{R,A}_R(E)\) has two components due to the coupling to the left and right contact. It replaces the boundary conditions that otherwise would be fulfilled by the construction of a Green function in the device region. The self-energy due to the left contact has the following expression:

\[
\Sigma^{R,A}_L(E) = V_{LD}g^{R,A}_L(E)V_{LD}^\dagger,
\] (13)

where \(g^{R,A}_L(E) = [(E \pm i\eta) - H_L]^{-1}\) is the Green function of the semi-infinite left contact. Also, \(\Sigma^{R,A}_R(E)\) has a similar expression. Here, we notice that due to the fact that we deal with a nearest-neighbor tight-binding Hamiltonian, the self-energies \(\Sigma^{R,A}_L\) and \(\Sigma^{R,A}_R\) are \(n_D \times n_D\) matrices with just one non-zero element, the \((1,1)\) element for \(\Sigma^{R,A}_L\) and \((n_D,n_D)\) for \(\Sigma^{R,A}_R\). Thus the retarded Green function is
The poles of the device Green function are no longer real, an attribute of an open quantum system. Starting from Eq. (13), the calculation of $\sigma_R^L(E)$ involves the calculation of matrix element $(0,0)$ of $g_R^L(E)$, which is the surface Green function of the left contact. Bearing in mind that $D_L$ and $t_L$ are the tight-binding parameters of the left contact and defining a longitudinal wavevector $k_L$, the energy can be parameterized according to the single-band dispersion relation for the left contact $E = D_L - 2t_L \cos (k_L \Delta)$. One can find that the matrix element $(0,0)$ of $g_R^L(E)$ is $-e^{ik_L \Delta}/t_L$ and $\sigma_R^L(E) = -t_L e^{ik_L \Delta}$ [14, 22, 27]. The expression of $g_R^L(E)$ is calculated with outgoing boundary condition [27], hence the self-energy is for this kind of boundary condition.

One can further define: (a) the spectral function $A = i (G^r - G^a)$, which also has a matrix form, whose diagonal is just local density of states up the $2\pi$ factor, and (b) the broadening function due to the coupling to the left and right contacts $\Gamma_{L,R}(E) = i \left( \Sigma_{L,R}(E) - \Sigma_{L,R}^\dagger (E) \right)$. Using the projection operator on the device $D$ one can show that the projection of the full spectral function $A$ on the device space is [28]

$$A_D(E) = i \left( G_D^R(E) - G_D^A(E) \right) = G_D^R(E) \left( \Gamma_L(E) + \Gamma_R(E) \right) G_D^A(E).$$  \hspace{1cm} (15)

Moreover one can further show that partial spectral densities

$$A_{L,R}(E) = G_D^R(E) \Gamma_{L,R}(E) G_D^A(E)$$  \hspace{1cm} (16)

are spectral densities due to incident Bloch waves that come respectively from the left (L) and from right (R) [28]. Thus $G_D^R(E)$ contains information about both solutions of the scattering problem. Furthermore it can be shown that the current flow from an incident Bloch wave that comes from the left electrode into the right electrode is
\[ j(E) = \frac{2e}{h} Tr \left[ G_D^R(E) \Gamma_L(E) G_D^A(E) \Gamma_R(E) \right] \]  

(17)

FIG. 2. The behavior of an incident Bloch wave \( \Psi_{nk+} \) coming from the left. A part is reflected with the coefficient \( r \) and the other part is transmitted with a coefficient \( t \). In the case of a single-band transport the coefficients \( r \) and \( t \) are simple scalars.

\[ G_D^R(E) \Gamma_L(E) G_D^A(E) \Gamma_R(E) \]  

is just the matrix of transmission probability \( T(E) \) that has a schematic representation in Fig. 2. From Eq. (17) the expression of the total current takes the form of Landauer-Büttiker formula [15, 22]:

\[ J = \frac{2e}{h} \int Tr (T(E)) (f_L(E) - f_R(E)) dE. \]  

(18)

In Eq. (18) the \( \text{Tr}() \) operation includes both the trace over the \( T(E) \) matrix and the integration over the transverse wavevector \( k \). The functions \( f_{L,R} \) are the Fermi-Dirac distribution functions of the \( L \) and \( R \) electrodes. Performing the trace operation only over matrix \( T \) we obtain the transmission probability coefficient \( \tilde{t} \) and the the Landauer-Büttiker formula becomes

\[ J = \frac{e}{2\pi^2 h} \int_{-\infty}^{\infty} d^2 k \int_{0}^{\infty} \tilde{t}(k,E) (f_L(E) - f_R(E)) dE. \]  

(19)

In addition, in the linear regime (small bias voltages \( V \)) and at temperature of 0K we obtain the Landauer conductance formula [15]

\[ G = \frac{2e^2}{h} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d^2 k_t}{(2\pi)^2} \tilde{t}(k_t, E_F). \]  

(20)
C. Retrieving the wavefunction from the spectral function. Resonance states

Let us consider the spectral function \( A_L(E) = G^R_D(E) \Gamma_L(E) G^A_D(E) \). It signifies the projected spectral function on the device for incident waves coming from the left. As it was pointed out in Ref. [28], in general the eigenvectors of \( A_L \) cannot be identified with the wavefunction in the device region since there are several eigenvectors of \( A_L \) with non-zero eigenvalues. This is rather obvious in the tight-binding representation but for multi-band problem. For a single-band problem, however, this is not the case. \( A_L \) has just one non-zero eigenvalue. Its corresponding eigenvector is just the function that is proportional to the wavefunction in the device region. This statement can be proven directly. The matrix \( \Gamma_L(E) \) has just one element different from 0 like its corresponding self-energies \( \Sigma^{R,A}_L(E) \)

\[
\Gamma_L(E) = \begin{pmatrix}
\gamma_L(E) & 0 & \cdots \\
0 & 0 & \\
\vdots & & \\
\end{pmatrix}.
\]

(21)

Denoting by \( G_{D,i,j}(E) \) the matrix elements of \( G^R_D(E) \) and by \( A_{L,i,j}(E) \) the matrix elements of \( A_L(E) \), it is easy to check that \( A_{L,i,j}(E) = \gamma_L(E) G_{D,i,1}(E) G^*_D,j,1(E) \), where the * means complex conjugation. One can further see that the \( n_D \)-dimensional vector

\[
v_L = \begin{pmatrix} G_{D,1,1}(E) & G_{D,2,1}(E) & \cdots & G_{D,n_D,1}(E) \end{pmatrix}
\]

(22)

is an eigenvector of \( A_L(E) \) with the eigenvalue

\[
\lambda_L = \gamma_L(E) \sum_{i=1}^{n_D} |G_{D,1,i}(E)|^2 = \text{Tr}(A_L(E)).
\]

(23)

The fact that \( \lambda_L = \text{Tr}(A_L(E)) \) ensures that \( \lambda_L \) is the only non-zero eigenvalue of \( A_L(E) \). In a bra and ket notation we thus write \( A_L(E) \) as

\[
A_L(E) = \gamma_L(E) |v_L\rangle \langle v_L|
\]

(24)

since the norm of \( v_L \) is just \( \sqrt{\lambda_L/\gamma_L} \). Eqs. (22) and (24) of \( v_L \) and \( A_L(E) \) guarantee that \( v_L \) is proportional to the solution of Schrödinger equation for incoming waves from the left projected on the device space
\begin{equation}
|\Psi_L\rangle_D = \sqrt{\frac{\gamma_L}{2\pi}} v_L
\end{equation}

Similar calculations can be performed for \( A_R(E) \), explicitly, the matrix form is 
\( A_{R,i,j}(E) = \gamma_R(E) G_{D,i,N}(E) G^*_{D,j,N}(E) \) with the eigenvector

\begin{equation}
v_R = \left( G_{D,1,n_D}(E) \ G_{D,2,n_D}(E) \cdots G_{D,n_D,n_D}(E) \right)
\end{equation}

the eigenvalue

\begin{equation}
\lambda_R = \gamma_R(E) \sum_{i=1}^{n_D} |G_{D,i,n_D}(E)|^2 = \text{Tr} (A_R(E)),
\end{equation}

and the simple bra and ket form

\begin{equation}
A_R(E) = \gamma_R(E) |v_R\rangle \langle v_R|.
\end{equation}

Also, Eqs. (26) and (28) of \( v_R \) and \( A_R(E) \) guarantee that \( v_R \) is proportional to the solution of Schrödinger equation for incoming waves from the right projected on the device space

\begin{equation}
|\Psi_R\rangle_D = \sqrt{\frac{\gamma_R}{2\pi}} v_R.
\end{equation}

The total spectral function \( A_D(E) \) is the sum of \( A_L(E) \) and \( A_R(E) \), hence its range is spanned by \( v_L \) and \( v_R \) with two eigenvalues \( \lambda_1 \) and \( \lambda_2 \). They obey the following equation:

\( \lambda_1 + \lambda_2 = \lambda_L + \lambda_R \). Also, it is easy to find that the squared modulus of the overlap between \( |\Psi_L\rangle_D \) and \( |\Psi_R\rangle_D \) is

\begin{equation}
|D\langle \Psi_L | \Psi_R\rangle_D|^2 = \frac{(\lambda_L \lambda_R - \lambda_1 \lambda_2)}{4\pi^2}.
\end{equation}

From the analysis we are going to perform in the next section on realistic examples we will see that for energies in the direct tunneling regime there are two distinct solutions with low overlap. In this case \( \lambda_1 \) and \( \lambda_2 \) are close to \( \lambda_L \) and \( \lambda_R \). In the opposite case, at resonance, one of the two eigenvalues \( \lambda_1 \) or \( \lambda_2 \) is much larger than the other, hence the overlap is large. In a similar manner we can obtain the explicit expression of the transmission probability in terms of the Green function

\begin{equation}
\tilde{t}(E) = \gamma_L(E) \gamma_R(E) |G_{D,1,n_D}|^2.
\end{equation}
Eq. (31) has been previously deduced using an iterative procedure to calculate the Green function \[22, 29\]. It additionally shows that the transmission probability has the spectral properties of the Green function.

There is a large body of work in which the Green function $G^R_D (E)$ is set in a meaningful representation. Such a representation is given by the expansion of the Green function in resonance (Siegert-Gamow) states $[23, 24]$, which lead to Breit-Wigner formula for resonances in transmission. Here we will outline a few results about resonant states representation that are connected with our results discussed above. The expansion of the Green function in resonance states is the sum over these states plus a background and it looks like the following

$$G^R_D (x, x', E) = \sum_{n=1}^{N} \frac{u_n (x) u_n (x')}{E - E_n} + B (E),$$

(32)

where $u_n (x)$ is a resonant state that satisfies the Schrödinger equation

$$H_D u_n (x) = E_n u_n (x)$$

(33)

with outgoing boundary conditions at the boundary of the device. Since these boundary conditions are not hermitian, the eigenvalues are rather complex, i. e., $E_n = E_{rn} - i\Gamma_n / 2$.

Resonant states come into pairs with a negative and positive imaginary part $[23, 25, 26]$. Now, it is rather obvious that for energy $E$ far from any resonant energy $E_{rn}$ the solution of Schrödinger equation for incoming waves from the left is different from the solution of the Schrödinger equation for incoming waves from the right due to different mixing of the tails of various resonances. However, for energy $E$ near a resonant energy $E_{rn}$ both solution from the left and from the right are similar since the dominant term is that given by $u_n (x)$. Finally, there is quite straightforward to notice by using Eq. (31) that transmission probability coefficient has a multi-resonance Breit-Wigner like form $[24]$

$$\tilde{t} (E) = \sum_{n=1}^{N} T_n (E) + \sum_{n<m}^{N} T_{nm} (E) + R (E).$$

(34)

The term

$$T_n (E) = \frac{A_n}{(E - E_{rn})^2 + (\Gamma_n / 2)^2}$$

(35)

is the Breit-Wigner expression, $T_{nm} (E)$ is the interference term between resonances, and $R (E)$ is the term resulting from the background.
III. NUMERICAL ANALYSIS OF TUNNELING IN RELEVANT FTJS

A. Temperature influence on conductance and TER ratio

Numerically we calculated all quantities defined in the previous section using NEGF formalism. The calculation of I-V characteristics is performed with Eq. (19), which is able to reproduce the non-linear regime for large bias voltages. Equation (20) describe the linear regime at 0K and is often used (especially in ab-initio calculations, where a full I-V curve is extremely costly) in the calculation of the TER ratio defined by Eq. (1). In the following we shall analyze a few practical FTJ structures.

![Figure 3](image)

FIG. 3. Potential profiles of a BaTiO$_3$ barrier of 2 nm thickness between Pt and SrRuO$_3$ metallic contacts for both directions of polarization. Schematically on the right hand side are shown the transmission probability coefficients.

1. Pt/BaTiO$_3$/SrRuO$_3$ FTJ

The first system to deal with is that of a BaTiO$_3$ ferroelectric barrier on top of a SrRuO$_3$ substrate which acts as contact layer, and on top of BaTiO$_3$ is the Pt contact, which is considered as the left contact. Physical parameters are: $\lambda_1 = 0.045$ nm, $\lambda_2 = 0.075$ nm, $\varepsilon_1 = 2$, $\varepsilon_2 = 8.45$, $\varepsilon_{FE} = 125$, $E_{FL} = E_{FR} = 3$ eV, $\phi_1 = \phi_2 = 3.6$ eV, $P = 16 \mu$C/cm$^2$. The effective masses are: 5 $m_0$ for SrRuO$_3$, 2 $m_0$ for BaTiO$_3$, and $m_0$ for Pt, where $m_0$ is the free electron...
The Fermi energy is set to $E_F = E_{FL} = E_{FR} = 3$ eV. One should note that the electron effective masses are different in the three layers of the structure, hence the calculations need full numerical integration over transverse $k$ wavevector in Eqs. [19] and [20]. In Fig. 3 we show the potential profiles of a 2 nm thick BaTiO$_3$ barrier for both directions of polarization. The transmission probability coefficients, also depicted in Fig. 3 right, exhibit resonances below and above the very top of the barriers. The resonances are associated with the peaks in the transmission spectra and if they are well resolved they obey Eq. (35). In Fig. 4(a) we plot the conductance of the system and in Fig. 4(b) the TER ratio at 0K and 300K.

FIG. 4. Pt/BaTiO$_3$/SrRuO$_3$ FTJ: (a) Conductance and (b) TER ratio as a function of the barrier thickness at 0K and 300K.

The calculation of the conductance at 300 K was performed with an applied bias of 0.0001 V which is low enough to satisfy the linear regime conditions. Both the conductance and TER ratio behave differently at 300K with respect to 0K. At 300K we observe two regimes depending on the ferroelectric thickness, one regime up to 2.5 nm and another one beyond that value. The difference between the two regimes is explained in Fig. 5. At 0K the channels open to electron flow are those up to Fermi energy represented by dashed line. These channels are those of direct tunneling such that the Simmons and Brinkman formulae are appropriate [17][19]. For the barrier of 1.6 nm thickness (Fig. 5(a)) the transport occurs around Fermi energy even at room temperature (300K), hence that similar behavior of the conductance at 300K with respect to 0K, see Fig. 4(a). There is a small contribution to the
transmitted current from the resonance states, but the contribution is orders of magnitude smaller. However, for thicker barriers, like the one shown in the Fig. 5(b) things may change. First, the direct tunneling current is much smaller since it has an exponential dependence on thickness. Second, the resonance levels are spaced much closer, hence their contribution increases considerably. Even if their occupancy, given by Fermi-Dirac function, might be small, it is offset by the large transmission probability. In Fig. 5(b) it can be easily seen that the contribution from resonance states is overwhelmingly larger than the contributions from states near the Fermi energy. Moreover, electrons with energies closer to the barrier top encounter a triangular barrier profile and so they may still reach a resonance state; this mechanism cannot be described within the semiclassical WKB theory of Fowler-Nordheim [21]. A similar behavior of the TER ratio at room temperature was also observed in experimental data [31]. It was found even a degradation of TER when increasing the ferroelectric thickness. However, performing their analysis based on Brinkman model at finite bias voltage, the authors attributed the TER degradation to the rather high levels of noise in the measurements.

FIG. 5. Pt/BaTiO$_3$/SrRuO$_3$ FTJ: the barrier profile, the transmission probability coefficient, and the Fermi-Dirac weighted transmission at 300K for two barrier thicknesses - (a) 1.6 nm and (b) 3.5 nm. The dashed line in the graphs indicates the Fermi energy.
2. \( \text{Pt/SrTiO}_3 / \text{BaTiO}_3 / \text{SrRuO}_3 \) composite barrier FTJ

The second system we analyze is a composite TFJ, where a dielectric barrier (SrTiO\(_3\)) is added beside the BaTiO\(_3\) ferroelectric barrier. The electrodes are Pt (left) and SrRuO\(_3\) (right). The role of the dielectric layer is to increase the asymmetry of the system, hence it is expected a higher TER ratio \[32\]. Physical parameters are slightly changed with respect the previous case \[32, 33\]: \( \lambda_1=0.045 \text{ nm}, \lambda_2=0.08 \text{ nm}, \varepsilon_1=2, \varepsilon_2=8.45, \varepsilon_{FE}=90, \varepsilon_{DE}=90, E_{FL} = E_{FR}=3 \text{ eV}, \phi_1=\phi_2=3.6 \text{ eV}, \phi_C=0 \text{ eV}, P=20 \mu \text{C/cm}^2 \). The effective masses are: 5 \( m_0 \) for SrRuO\(_3\), 2 \( m_0 \) for BaTiO\(_3\) and SrTiO\(_3\), and \( m_0 \) for Pt. In the following, BaTiO\(_3\) thickness is fixed to 2.4 nm and we have varied the SrTiO\(_3\) thickness from 0.5 nm to 3 nm. The results of calculations are presented in Fig. 6.

![FIG. 6. Pt/BaTiO\(_3\)/BaTiO\(_3\)/SrRuO\(_3\) composite FTJ: (a) Conductance and (b) TER ratio as a function of the dielectric thickness at 0K and 300K.](image)

At 0K the conductance for both polarization directions shows an exponential dependence on dielectric thickness. At room temperature, on the other hand, it appears that this exponential dependence is no longer valid, as revealed by the TER ratio. In this case, a decrease of TER ratio takes place when the dielectric thickness increases (Fig. 6(b)). The explanation of TER degradation is provided by the results presented in Fig. 7. One may observe that the electric charges are mainly transported through quantum states that are close or above the barrier top, the contribution of the states near the Fermi energy being negligible. The total barrier thickness is 3 nm at least, a value at which the resonance states
start to play a significant role. As the barrier thickness is increased the contribution of the resonance states is enhanced. Nevertheless, those resonances located above the barrier (see the Fermi-Dirac weighted curves in Fig. 7) become less sensitive to barrier profile and hence the decline of TER ratio with barrier thickness increase.

![Graph](image_url)

**FIG. 7.** Pt/SrTiO$_3$/BaTiO$_3$/SrRuO$_3$ composite FTJ: the barrier profile, the transmission probability coefficient, and the Fermi-Dirac weighted transmission probability at 300K; $t_{FE}$=2.5 nm, $t_{DE}$=1 nm. The dashed line in the graphs indicates the Fermi energy.

3. **Metal/ CaO/BaTiO$_3$/Metal composite FTJ**

The third system studied herein is also a composite TFJ, with a CaO dielectric barrier added to the BaTiO$_3$ ferroelectric barrier. The electrodes are of the same generic metal Me. In this case the asymmetry is ensured just by the presence of dielectric. We have set the the physical parameters to $^{[32]}$: $\lambda_1 = \lambda_2 = 0.1$ nm, $\varepsilon_1 = \varepsilon_2 = 1$, $\varepsilon_{FE} = 90$, $\varepsilon_{DE} = 10$, $E_{FL} = E_{FR} = 3$ eV, $\phi_1 = 5.5$ eV, $\phi_2 = 3.6$ eV, $\phi_C = 1.9$ eV, $P = 40 \mu$C/cm$^2$. The effective masses are equal to $m_0$ for all materials. We have also kept the thickness of BaTiO$_3$ to 2.4 nm and we have varied the thickness of CaO from 0.5 nm to 3 nm. In comparison to the previous system, in this particular case the barrier is much higher on the dielectric side. The calculations of conductance and TER ratio are presented in Fig. 8.

In contrast to Pt/SrTiO$_3$/BaTiO$_3$/SrRuO$_3$, the conductance and the TER ratio of Me/CaO/BaTiO$_3$/Me composite FTJ exhibit an exponential dependence on dielectric thickness at both 0K and 300K. Therefore, qualitatively at least, a 0K analysis remains valid.
also at room temperature. In Fig. 9 we show the data for a quantitative explanation of conductance and TER ratio behavior with temperature. One can see that resonance states have a minor contribution to the current; the vast majority of carriers are transported through states around Fermi energy, although there are many resonances below the top of the barrier. Due to the higher dielectric barrier, these resonance states are just weakly coupled to the contacts, hence they show low transmission coefficients and they have a modest contribution to conductance.

B. The tunneling wavefunctions. The wavefunctions of resonances

In the previous section it was discussed that the energy dependent transmission in FTJs has resonant features besides an exponential background. In this section we show that the wavefunctions also exhibit general features, some of which, e. g., those corresponding to resonances, are also observed in other nanostructures like quantum wells, multi-barrier structures, etc. Usually, as a scattering problem, the electron transport in FTJs has two solutions at a given energy: one solution for an incident electron wave coming from the left and the other for the electron wave coming from the right. In the following we will illustrate the wavefunctions at some representative energy values for two FTJs: Pt/BaTiO$_3$/SrRuO$_3$ and Pt/SrTiO$_3$/BaTiO$_3$/SrRuO$_3$
FIG. 9. Me/CaO/BaTiO$_3$/Me composite FTJ: the barrier profile, the transmission probability coefficient, and the Fermi-Dirac weighted transmission probability at 300K; $t_{FE}=2.5$ nm, $t_{DE}=0.5$ nm. The dashed line in the graphs indicates the Fermi energy.

1. The wavefunctions of Pt/BaTiO$_3$/SrRuO$_3$ FTJ

We illustrate the wave functions at Fermi energy (3 eV) and at some resonant energies like that can be taken from Fig. 10.

FIG. 10. Transmission probability coefficient for a BaTiO$_3$ barrier of 1.6 nm thickness between Pt and SrRuO$_3$ metallic contacts for both polarization directions.

It is obvious that up to about 3.5 eV the transmission probability has an exponential dependence with respect to energy. In Fig. 11 we plotted the wavefunctions of a 1.6 nm thick...
BaTiO$_3$ barrier at Fermi energy as well as the first few resonance energies for both directions of polarization. In order to compare those wavefunctions we plotted the “normalized” eigenvectors of $A_L$, $A_R$, and $A_D$. In other words, for instance, $|\Psi_{L,R}\rangle_D$ are divided by $\sqrt{\lambda_{L,R}/2\pi}$ and the eigenvectors of $A_D$ are divided by $\sqrt{\lambda_{1,2}/2\pi}$ with $\lambda_{1,2}$, the corresponding eigenvalues.

The device region is comprised of the barrier and several layers of contact regions, such that the region outside the device should exhibit a flat electrostatic potential. In practice this is achieved when a few nanometers of contacts are added to device region. At Fermi energy the wavefunctions are almost real and their overlap is almost zero. They decay exponentially in the barrier, hence the Simmons or Brinkman formula applies for states around Fermi energy.

Since the barrier is thin the resonances are well separated. From Figs. 11(a), 11(b) and Figs. 11(d), 11(e) we see that the “normalized” $|\Psi_L\rangle_D$ is almost identical with the complex conjugation of “normalized” $|\Psi_R\rangle_D$, however the values of $\lambda_{L,R}/2\pi$ provide the levels of electron density inside the device for the corresponding wavefunction. These states exhibit a confining character within the barrier, in contrast to the states shown at Fermi energy. These solutions belong to resonance and anti-resonance states in the complex wavevector plane [23, 25, 26]. Moreover, the real and the imaginary parts of $|\Psi_{L,R}\rangle_D$ can be found in the normalized eigenvectors of $A_D$ (Figs. 11(c) and 11(f)). Finally, by analyzing Figs. 5 and 11 we notice that just the first resonance would participate to the electron transport at room temperature.

2. The wavefunctions of Pt/SrTiO$_3$/BaTiO$_3$/SrTiO$_3$ composite FTJ

The plots of the wave functions for this composite FTJ are shown in Fig. 12. The transmission probability for polarizations is shown in Fig. 12(a) from which we can extract the resonances that play a role in the electron transport at room temperature. The physical parameters are those that have already been used in the calculations. The effective thickness of the barrier is larger than in simple FTJ presented in the previous subsection; hence the resonances are closely spaced. Still, at Fermi energy the wavefunctions decay exponentially in the barrier and are almost real, while their overlap is almost zero. The wavefunctions of the first four resonances in transmission have a much smaller imaginary part, which is not shown here. Like in the previous section, these wavefunctions manifest confining character.
FIG. 11. Representative wavefunctions of BaTiO$_3$FTJ as normalized eigenvectors of $A_L$ (solid black line), $A_R$ (dotted red line). They are scaled down by a factor $\sqrt{\lambda_{L,R}/2\pi}$, where $\lambda_{L,R}$ is the corresponding eigenvalues of $A_L$, $A_R$. In addition we illustrate the normalized eigenvectors of $A_D$ with eigenvalue $\lambda_1$ (solid black line) and $\lambda_2$ (dotted red line). The normalized eigenvectors of $A_L$, $A_R$ are as follows: (a) - real part, positive ferroelectric polarization; (b) - imaginary part, positive ferroelectric polarization; (d) - real part, negative ferroelectric polarization; (e) - imaginary part, negative, ferroelectric polarization. The normalized eigenvectors of $A_D$, are as follows: (c) - positive ferroelectric polarization; (f) - negative ferroelectric polarization.
in the barrier. Moreover, the dielectric induces a much smaller coupling to one of the two contacts, such that the first two resonances in transmission contain a significant background contribution as a decaying wavefunction in the barrier seen in the solution from the left (Fig. 12(b), positive polarization) and in the solution from the right (Fig. 12(d), negative polarization). Analyzing Figs 12(c) and 12(e) one can notice that the overlap between the solution from the left and that from the right is almost zero for the first two resonances in transmission. The next two resonances in transmission, however, can be distinguished from the background, the normalized eigenvectors of $A_L$ and $A_R$, being quite similar, yet the corresponding wavefunctions $|\Psi_L\rangle_D$ and $|\Psi_R\rangle_D$ have quite different amplitudes. The difference in amplitudes starts to close in as we move to higher energies, since at sufficiently higher energy the asymmetry of the barrier will not play any major role in the electron transmission. As a final comment, all four resonances shown here participate to temperature activated transport (Fig. 7). However, the main contribution to temperature dependent transport is given by the first three resonances, even though the couplings to the contacts of the first two resonances are not so strong as the couplings of the third one which is further apart in energy.

IV. CONCLUSIONS

In conclusion, the semi-empirical model of electrostatic and NEGF calculations can provide a detailed picture of electron transport in systems with FTJs. It treats on equal footing several transport mechanisms that are usually invoked when studying these devices like direct tunneling, thermionic emission, and Fowler-Nordheim tunneling. This feature of NEGF allows us to assess in detailed form the role of temperature in electron transport and how temperature affect TER ratio. We have found that for simple or composite BaTiO$_3$ based FTJs the transport through temperature activated resonance (Gamow-Siegert) states may become dominant, affecting both the conductance and the TER ratio; thus, the more resonances are activated and the stronger their couplings to the contacts the more powerful is the effect of temperature. The effect of temperature is obvious in thicker FTJs, since the resonance states, especially those above the barrier, are closer to each other, hence more of them may participate in the transport. More insides into this phenomenology may be acquired by calculating and plotting the wavefunctions at any given energy. We show that
FIG. 12. Pt/SrTiO$_3$/BaTiO$_3$/SrTiO$_3$ composite FTJ (1 nm of SrTiO$_3$ and 2.4 nm of BaTiO$_3$). (a) Transmission probability for positive (dotted red line) and negative (solid black line) ferroelectric polarization; (b)-(e) Like in Fig. 11 the representative wavefunctions are the normalized eigenvectors of $A_L$ and $A_R$ as well as the normalized eigenvectors of $A_D$. The real part of normalized eigenvectors of $A_L$ (solid black line) $A_R$ (dotted red line) are as follows: (b) - positive ferroelectric polarization; (d) - negative ferroelectric polarization. The normalized eigenvectors of $A_D$ with eigenvalue $\lambda_1$ (solid black line) and $\lambda_2$ (dotted red line) are as follows: (c) - positive ferroelectric polarization; (e) - negative ferroelectric polarization.
this is possible for NEGF calculations of single-band transport. Thus the transport by direct tunneling is made through states whose wavefunctions have a decaying shape in the barrier. These states belong to the background generated by all resonance states. Furthermore, where the resonances are strong and well separated, the wavefunctions show confinement character in the barrier. In the intermediate regime, where the resonances are weak, the confining character of the resonance competes with the decaying character of the background. Lastly, we suggest that these thorough insights can be used in the optimization process of the FTJ design in various applications, particularly at high temperature.

Appendix A: The BenDaniel and Duke Hamiltonian

The BenDaniel and Duke Hamiltonian

\[ H = -\frac{\hbar^2}{2} \frac{d}{dx} \left( \frac{1}{m^* (x)} \frac{d}{dx} \right) + \frac{\hbar^2 k^2}{2m^* (x)} + U (x) \]  

can be cast into 1D problem by rewriting it as

\[ H = -\frac{\hbar^2}{2} \frac{d}{dx} \left( \frac{1}{m^* (x)} \frac{d}{dx} \right) + V_k (x) + \frac{\hbar^2 k^2}{2m^*_L}, \]  

where \( m^*_L \) is the effective mass in the left contact and

\[ V_k (x) = U (x) + \frac{\hbar^2 k^2}{2m^*_L} \left( \frac{m^*_L}{m^* (x)} - 1 \right). \]

Equation (A2) is discretized and its discrete form can be mapped into a tight-binding Hamiltonian. Thus the continuous variable \( x \) is transformed in the discrete version \( \Delta \cdot n \), where \( \Delta \) is the discretization step and \( n \) is an integer running from \( -\infty \) to \( \infty \). We define a localized orbital \( |n, R^L\rangle \) with \( \Delta \cdot n \) and \( R^L \) as longitudinal and transverse positions. Moreover, we construct transverse Bloch orbitals as a sum over \( N \) localized orbitals in the transverse plane

\[ |n, k\rangle = \frac{1}{\sqrt{N}} \sum_{R^L} e^{ikR^L} |n, R^L\rangle. \]

In this Bloch basis the Hamiltonian has the following expression

\[ \langle n, k | H | n', k \rangle = D_n (k) \delta_{n,n'} - t_{n,n'} \delta_{n,n\pm1}, \]
where

\[ D_n(k) = \frac{\hbar^2}{2\Delta^2} \left( \frac{1}{m^-} + \frac{1}{m^+} \right) + V_k(n), \quad (A6) \]

\[ t_{n,n'} = \frac{\hbar^2}{(m_n^* + m_{n'}^*) \Delta^2}, \quad (A7) \]

\[ m^- = \frac{m_{n-1}^* + m_n^*}{2}, \quad (A8) \]

\[ m^+ = \frac{m_n^* + m_{n+1}^*}{2}. \quad (A9) \]

The tight-binding version \([A5]\) of BenDaniel and Duke Hamiltonian has a tridiagonal form. The left contact is defined for \( n \) running from \(-\infty\) to 0, the device is defined for \( n \) running from 1 to \( n_D \), and the right contact from \( n_D + 1 \) to \( \infty \). The left and the right contacts are homogeneous systems; hence we define the tight-binding parameters as follows. The diagonal term of the left (right) contact is defined as \( D_L (D_R) \), while the off-diagonal terms \( t_{i,i\pm1} \) as \( t_L (t_R) \).

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