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Study on Electron Tunneling Lifetime by Projected Green's Function Approach in Single Quantum Well Semiconductor

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ABSTRACT

The tunnelling lifetime of an electron in a single quantum well subject to an externally applied electric field is calculated using the Projected Green's Function (PGF) approach. The lifetime in the biased single well decreases as a function of the electric field in good agreement with the previous result. The tunnelling lifetime is revealed with the behavior of the ground-state shift and the wave amplitude in the first well. As the electric field increases, the ground state energy shifts, leading to lessened constructive interference between the initial and reflected electron waves. Consequently, the study is essential to characterize the performance of high-speed quantum devices.

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1. INTRODUCTION

Investigating a tunneling lifetime in quantum heterostructures has become an interest in the semiconductor industry. The tunneling escape of a carrier from a quantum well (QW) is one of the main aspects that affect the performance of a QW-based electronic device (Chan & Zhang, 1998; Moss, Ido, & Sano, 1994; Tsuchiya, Matsusue, & Sakaki, 1987). In the strong field ionization, the lifetime of the bound state was computed and found to be in perfect agreement with the Bohmian time (Zimmermann, Mishra, Doran, Gordon, & Landsman, 2016). In application, the tunneling lifetime characterizes the performance of high-speed quantum devices (Harditya, 2019; Shahriar et al., 2020), which are now commonly used, such as high-speed resonant tunneling diodes and optical switching devices (Li, Gong, Hu, & Zhang, 2010). Their response is determined when an electron continues to be confined inside the heterostructure at a particular energy eigenvalue. Therefore, to

optimize the performance of these quantum devices, the tunneling lifetime needs to be accurately calculated.

Several approaches have been proposed for the tunneling lifetime calculation like the phase shift method (Austin & Jaros, 1985), the stabilization method (Borondo & Sanchez-Dehesa, 1986), the orthogonalization approach (Ahn & Chuang, 1986), the Airy function approximation (Ghatak, Goyal, & Gallawa, 1990), the argument principle theorem (Anemogiannis, Glytsis, & Gaylord, 1993), and the Projected Green's Function (PGF) (Chan & Zhang, 1998; Li et al., 2010; Tao, Zhao, Sarwono, & Zhang, 2017; Zhao, Sarwono, & Zhang, 2017). The PGF approach is proven very effective in the tunneling lifetime calculations of QWs (Li et al., 2010; Tao et al., 2017) and atoms (Zhao et al., 2017). The approach showed how splitting a barrier into several thinner barriers influences the tunneling lifetime of an electron (Li et al., 2010; Tao et al., 2017). Later the PGF approach was extended to calculate the tunneling lifetime of an electron from a series of atoms like He, Ne, Ar, Kr, revealing the effect of the bound strength of the ground state electron on the escaping lifetime (Zhao et al., 2017). However, the calculation of the tunneling lifetime of the biased single quantum well has not previously been performed with PGF, although such cases are common in the study of electronic devices.

The present work uses the PGF method to address the electron tunneling lifetime in the biased single QW. Section 2 briefly discusses the theory of the PGF, while Section 3 shows the results of applying the PGF method on the biased single QW tunneling lifetime calculation. A model structure is given, and then the comparison is made with the previous result. We write our conclusion in Section 4.

2. RESEARCH METHODOLOGY

Consider an ideal electron initially localized in a one-dimensional potential well and described by a state $|\phi, t_0\rangle$. The electron is a spinless and non-interacting one. The effect of temperature and the influence of any other field is neglected. When an external field F is turned on, the initial state becomes a quasibound state and gradually reaches a stable final state $|\phi, t_0; t\rangle$.

The Hamiltonian with the included external field F along x direction is expressed as

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - eFx \qquad (1)$$

Where m and e are the electron's mass and the charge, respectively. The potential energy $V(x)$ as a function of the position is zero inside the well. V_0 is the finite barrier height. The initial electron state is expressed as a linear superposition of the energy eigenstate $|\emptyset t_0\rangle = \sum_j c_j |\psi_j, t_0\rangle$, which is carried out by initially putting the electron in a biased single well structure, shown in **Figure 1**.

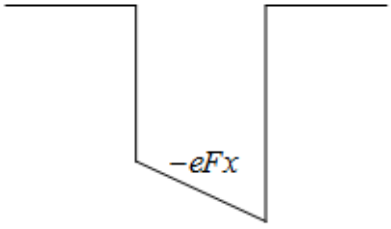

Figure 1. The localized and biased single well structure where an electron is located initially. The biased single well generates the eigenstate through the linear combination of the Airy functions.

The eigenstate $|\psi, t_0\rangle$ satisfied both Equation (1) and the boundary conditions $\langle x = 0|\psi, t_0\rangle = \langle x = L|\psi, t_0\rangle = 0$ for the heterostructures length L, obtained numerically from the structure of the localized-biased single well. $|\psi, t_0\rangle$ is in the linear combination of the Airy function $A_i(z)$ and its complement $B_i(z)$ for the new coordinate system $z = (2meF/\hbar^2)^{1/3}\left(x - \frac{E}{eF}\right)$ (Ghatak et al., 1990). The final electron state is expressed as $|\phi, t_0; t\rangle = \theta(t)\sum_j c_j e^{-iE_j t/\hbar}|\psi_j, t_0\rangle$, where $\theta(t)$ is the Heaviside step function. The introduced step function ensures the evolution of the electron at $t \geq 0$. The expansion coefficient evolves as a function of time with the unchanged modulus.

The total tunneling lifetime in the projected Green's function (Chan & Zhang, 1998; Li et al., 2010; Tao et al., 2017; Zhao et al., 2017) is given as

$$\tau_\delta = \frac{\hbar}{2\delta}, \tau = -\frac{\hbar}{2b_1^2\, Im\, G_1(E)}. \quad (2)$$

The projected Green's function (PGF) is initially proposed by Chan and Zhang (Chan & Zhang, 1998) to measure the lifetime when an electron is initially localized in a quantum well and then escapes to a bulk region, a situation which is not easily solved with the existing methods (Anemogiannis et al., 1993; Ghatak et al., 1990) due to the incoherent of the electron wave function throughout the whole quantum well structure. Using the recursion method, the projected Green's function is expressed as a continued fraction with coefficients a_i and b_i. In Equation (2), δ is a small imaginary part ensuring the convergence of the integral interpreted physically as the effect of scattering by impurities or phonons. The b_1 is the first recursive coefficient located in the lower diagonal in the first continued fraction G_1. Based on Equation (2), the inelastic scattering decay time τ_δ through the imaginary potential (Asada, 1989), and the tunneling lifetime τ through the barrier provide two parallel and independent channels for the total tunneling lifetime τ_t, related as $\frac{1}{\tau_t} = \frac{1}{\tau_\delta} + \frac{1}{\tau}$. The contribution of τ_δ is essential to reduce the total tunneling lifetime from the infinite to the finite time despite the inescapability of the electron from the confining barriers. The two independent channels of Equation (2) are comparable to Equation (6) of (Lefebvre & Anwar, 1997), where the escaping electron from the biased single quantum well occurs through two paths of the current components, namely the thermionic emission current and the tunneling current.

3. RESULTS AND DISCUSSION

A model structure illustrated in the inset of **Figure 2** consists of a WQ with a width of 96 Å flanked by two barriers and a width of 200 Å. The results are plotted in **Figure 2** and compared to a formerly reported theoretical study (Lefebvre & Anwar, 1997). Throughout the calculation, the delta, which accounts for the scattering of phonons and impurities, was set to 5 meV (Asada, 1989), and the 0.1 effective electron mass was adopted following the former theoretical studies (Chan & Zhang, 1998; Li et al., 2010; Tao et al., 2017; Zhao et al., 2017). The quantum well is asymmetric due to the different compositions of Al, which are 40% and 20% in the first and second barriers, respectively. The material parameters for the conduction band offset of $Al_{0.4}Ga_{0.6}As$ and $Al_{0.2}Ga_{0.8}As$ are 0.3242 eV and 0.1621 eV, respectively (Lefebvre & Anwar, 1997). The result of our calculation is shown in **Figure 2,** along with the previously reported theoretical result, which investigated the escape time of an electron in the case of two 200 Å-AlGaAs barriers and one 96 Å-Ga As well (Lefebvre & Anwar, 1997).

The results from the PGF method demonstrated in **Figure 2** show an excellent agreement with the unweighted tunneling escape time reported in previous work (Lefebvre & Anwar, 1997) which has been demonstrated to be in excellent agreement with the experimental data of the carrier escape time due to the applied field accounting the factors of the density states, the group velocity, and the partition between the tunneling and the thermionic components of current. In the absence of the bias voltage, our calculated value for the tunneling lifetime of the electron is 1.19 ms. Although there is no true bound state in our finite square well potential with a big value of barrier thickness, in zero electric fields, the remnant of the bound state is seen here with a large number of the electron tunneling lifetime. The energy of the electron in this state is the same as the energy of the electron located in the initial potential, which will be discussed in the next paragraph, so the energy is not or narrowly spread into a range of $\hbar/\tau$, where τ is the lifetime.

The lifetime time scale in the low electric field region (<20 kV/cm) drops to around a hundred picoseconds. The less rectangular barrier leads to a higher transmission coefficient. In a strong electric field ($> 20\ kV/cm$), the lifetime time scale is around a few picoseconds – the more triangular barrier results in a higher transmission coefficient. This shows that the quasibound state broadly spreads its energy into a range of $\hbar/\tau$, resulting in a shorter lifetime.

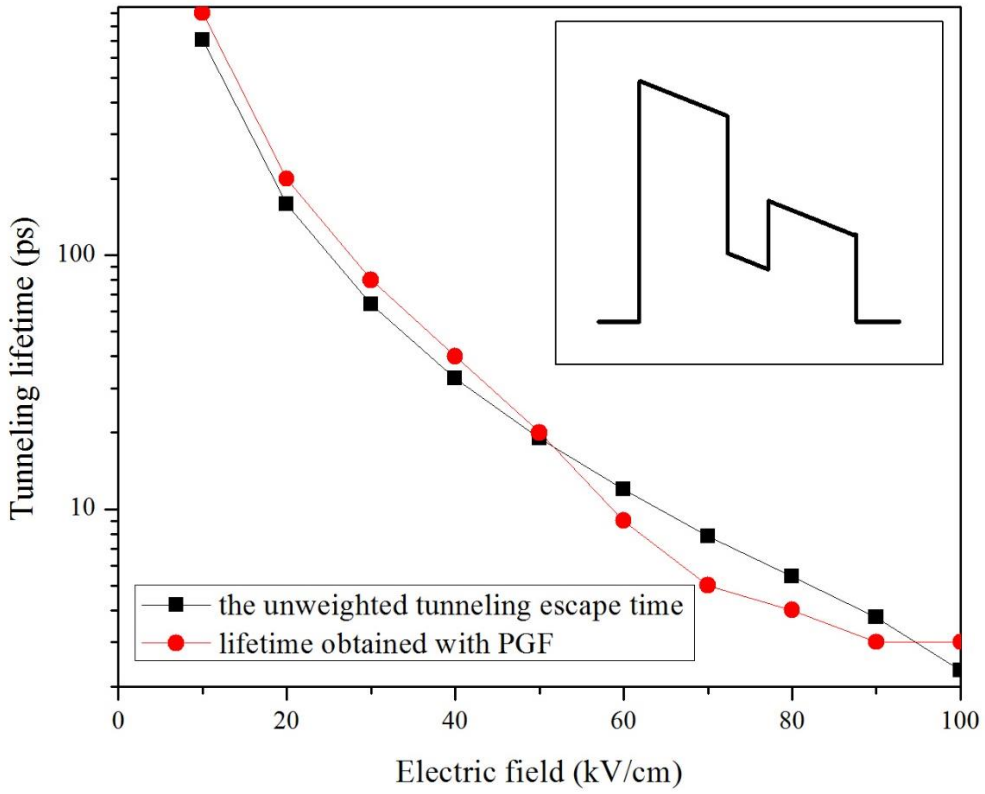

Figure 2. The tunneling escape time (black line with square knots) from the previous theoretical results (Lefebvre & Anwar, 1997) and the tunneling lifetime (red line with circular knots) obtained using the PGF approach. The inset shows our model of the biased single quantum well potential structure. The present results confirm the general trend of the decrease of the lifetime as the increase of the field.

Variation analysis of the parameters b_1 and $\mathrm{Im}\, G_1$ in Equation (2) reveals the underlying physics of the process. **Figure 3** shows b_1 as a function of the applied electric field. In the biased single well, b_1 is a linear function of the external electric field and is a measure of the initial electron-wave function ground state energy shift. When the barrier is rectangular, with no applied bias voltage, the value of b_1 is zero. The ground state energy of the initial electron wave function does not experience the shift, and the remnant of the electron-bound state stays in the well for a long time. As the electric field increases and the shape of the barrier becomes more triangular, the value of b_1 linearly increases. As a function of the external field, the $\mathrm{Im}\, G_1$ is maximum when there is no applied voltage since the electron wave function, in this case, is located inside the single well, shown in **Figure 3**.

The reflected electron waves from the left and the right barrier interfere constructively. With the increase of the applied bias voltage, the amplitude of the electron wave found in the well suddenly decreases, indicated by the lessened $Im\, G_1$. Destructive interference between the reflected electron waves occurs. As expected, the $Im\, G_1$ values in the presence of the bias voltage never return to the maximum value of the $Im\, G_1$ at no applied bias voltage.

Note that within the considered range of energy, the value of the $Im\, G_1$ is a constant, leading to a clear Lorentzian peak of the imaginary part of the PGF ($Im\,\mathrm{PGF}$). If the $Im\, G_1$ is not constant within the range of energy considered, the $Im\,\mathrm{PGF}$ will not show a Lorentzian peak, and the calculation of the tunneling lifetime with the PGF approach is invalid (Chan & Zhang, 1998; Li et al., 2010; Tao et al., 2017; Zhao et al., 2017).

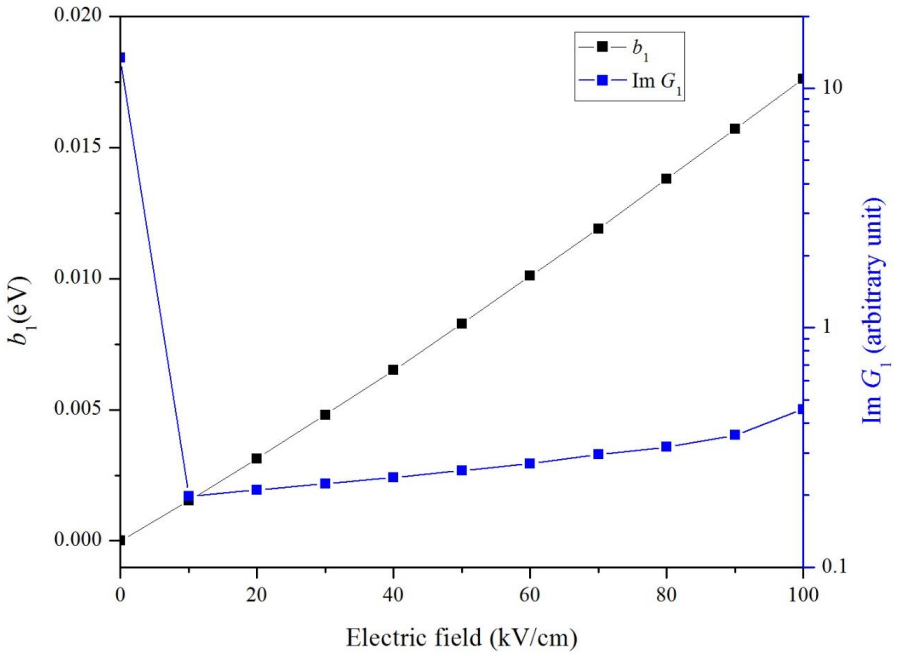

Figure 3. The coupling constant b_1 and the ImG_1 as a function of the electric field in the case of a biased single well. b_1 indicates the ground state energy shift of the initial electron wave function in the well, increasing linearly as the increase of field. ImG_1, associated with the wave amplitude of the electron in the well, is maximum when no applied bias voltage due to constructive interference. The presence of the applied bias voltage decreases the amplitude of the electron wave found in the well, causing destructive interference that the value of ImG_1 never returns to the value at no applied bias voltage.

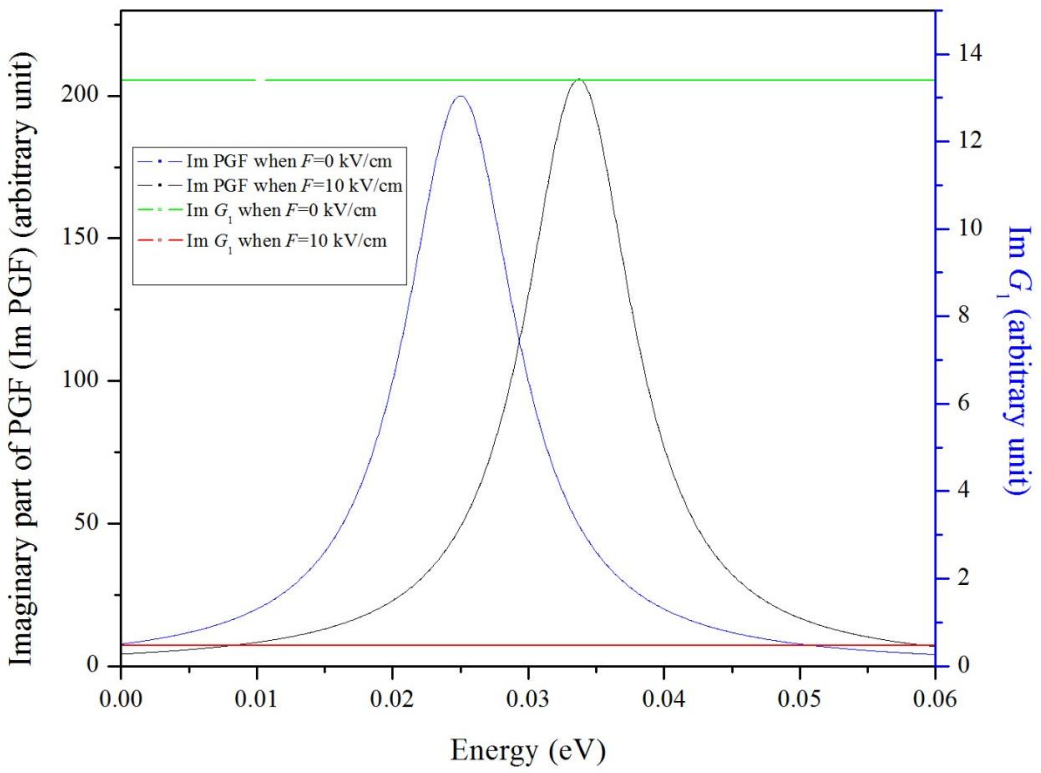

Figure 4. The imaginary part of the PGF and the *ImG₁* for two cases of the bias voltage F=0 kV/cm and F =10 kV/cm. The two values of the *ImG₁* are constant within the energy considered. The *Im* PGF exhibits a clear Lorentzian peak.

Figure 4 shows the ImG_1 and the Im PGF for two different values of electric field $F = 0\ kV/cm$ and $F = 10\ kV/cm$. The $Im\,G_1$ are constant in the two considered cases. Furthermore, the Im PGF shows the Lorentzian peak. The center of the peak is shifted following the resonant energy. The peak as a function of the $Im\,G_1$ becomes localized with the increased applied bias voltage.

4. CONCLUSION

In the present work, the resonant tunneling lifetime of an electron in the biased single well is calculated using the projected Green's function (PGF) approach. In agreement with the former theoretical result, the estimated lifetime decreases. The coupling constant b_1 and the $Im\,G_1$ reveal the physics in the tunneling lifetime. The value b_1 is related to the ground state energy shift of the initial electron wave function in the first well and responds almost linearly as a function of the applied electric field. The $Im\,G_1$ accounts for the wave amplitude of the electron in the first well.

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