Resonances in Fock Space: Optimization of a SASER device

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Abstract

We model the Fock space for the electronic resonant tunneling through a double barrier including the coherent effects of the electron-phonon interaction. The geometry is optimized to achieve the maximal optical phonon emission required by a SASER (ultrasound emitter) device. PACS numbers: 73.20.Dx, 73.40.Gk, 73.50.Rb

The possibility of generating coherent phonons in a double barrier semiconductor heterostructure was first proposed\cite{1} a few years ago. This is the basis of a SASER device\cite{2} which transforms the electric potential energy in a single vibrational mode of the lattice. This is facilitated by the electronic confinement in a double barrier structure. The phonon emission appears when the energy of the resonant state is one quantum $\hbar\omega_0$ (LO phonon energy) bellow the energy of the incoming electrons. As in laser devices this is enhanced if the first excited state of the well lies bellow the Fermi energy and becomes overpopulated. According to ref.\cite{3} the emitted LO phonons decay coherently into a pair of LO and TA phonons the last the useful ones in a SASER device.

In this paper we want to explore the case in which well’s ground state mediates the decay of the emitter states into the collector’s ones plus a phonon. This feature represents a resonance in the electron-phonon Fock space and is observed as a satellite peak in the current\cite{4}. This resonant condition is tuned directly by the applied voltage and we expect that its optimization could also provide enough emission of primary phonons to allow for SASER operation. We carry out the modeling of the electronic structure and the electron-phonon interaction to get a minimal structure in the Fock space. Thus, the optimization of the phonon emission for different geometries of the device (height and width of the barriers, field intensity) can be discussed in simple terms.

We consider a one-dimensional model for a double barrier including the inter-
action with LO phonons in the well, neglecting the effects derived from the accumulated charge. This will give results comparable to the 3-D case when \( \varepsilon_F \) is small, thus limiting the number of traversal modes; or in the presence of a high magnetic field perpendicular to the plane of the barriers[5] which quantize these modes in Landau levels. We do not consider the phonon-phonon interaction that leads to the decay of the LO phonons.

The Hamiltonian is a sum of an electronic contribution, a phonon contribution and an electron-phonon interaction term.

\[
H = H_e + H_p + H_{e-p}
\]

\[
H_e = \sum_j E_j c_j^+ c_j - \sum_{j,k} V_{j,k}(c_j^+ c_k + c_k^+ c_j),
\]

\[
H_p = \hbar \omega_0 \sum_{k[\text{well}]} b_k^+ b_k, \quad \text{and} \quad H_{e-p} = V_g \sum_{k[\text{well}]} c_k^+ c_k(b_k^+ + b_k).
\]

where \( c_j^+ \) and \( c_j \) are electron operators on site \( j \), \( E_j \) is the site dependent diagonal energy and \( V_{j,k} = V \delta_{j, \pm 1,k} \) are the hopping parameters. We assume that the potential drop \( eV \) is linear through the double barrier and limited to it. \( N_L \) and \( N_R \) are the number of sites in the left and right barriers and \( N_w \) are those in the well, the associated lengths are \( L_i = N_i \times 2.825 \text{Å} \). There is a single well state in the energy range of interest.

Since the most important interaction between electrons and phonons in polar semiconductors involves longitudinal optical (LO) phonons, only one phonon mode with frequency \( \omega_0 \) is considered. The electron-phonon interaction is limited to the well region and the coupling to the phonons is denoted with \( V_g \). The model is represented schematically in figure 1.

For simplicity we restrict the problem to the case in which we have either 0 or 1 phonons with no phonons in the well before the scattering process. By modifying \( V_g \to V_g \sqrt{n + 1} \) this also represents a finite temperature emission
Fig. 2. Inelastic current as a function of the applied voltage for different values of NR.

$n \rightarrow n+1$. The effective mass is taken to be \(0.067 \, m_e\), the LO phonon frequency \(\hbar \omega_0 = 36 \, \text{meV}\) and the value of the hopping parameter \(V = -7.1018 \, eV\). \(V_g\) is taken 10meV which gives a typical electron-phonon interaction strength \(g = (V_g/\hbar \omega_0)^2 \simeq 0.1\). The barrier heights are 300meV and the Fermi energy \(\varepsilon_F\) is taken between 10 and 20 meV.

This discrete model is solved exactly using a decimation procedure for the sites in the barriers and the well [6]. The leads are taken into account by adding a proper self-energy. The transmittances are computed from the Green’s functions for the system [7].

Let us denote with \(T_{0,0}^{R\leftarrow L}(T_{0,0}^{L\leftarrow R})\) and \(T_{1,0}^{R\leftarrow L}(T_{1,0}^{L\leftarrow R})\) the transmission coefficients from left (right) to right (left) where the subscripts 0 and 1 denote the number of phonons in the outgoing (first subscript) and in the incoming (second subscript) channel. The total current is a sum of an elastic current \(I_{el}\) and an inelastic current \(I_{in}\) (with the emission of one phonon during the scattering process). These currents can be calculated from the following expressions

\[
I_{el} = \frac{2e}{h} \int \left[ T_{0,0}^{R\leftarrow L} f_L(\varepsilon) - T_{0,0}^{L\leftarrow R} f_R(\varepsilon) \right] \, d\varepsilon,
\]

\[
I_{in} = \frac{2e}{h} \int \left[ T_{1,0}^{R\leftarrow L} f_L(\varepsilon) - T_{1,0}^{L\leftarrow R} f_R(\varepsilon) \right] \, d\varepsilon;
\]

where \(f_L(\varepsilon)\) and \(f_R(\varepsilon)\) are the Fermi functions for the left and right leads.

For a given configuration of the system a curve of inelastic current vs. applied bias is obtained and its maximum value \(I_{in}^{max}\) can be extracted. Figure 2 shows \(I_{in}=V\) curves as we change \(N_R\). The peaks in these curves correspond to the inelastic contributions to the main peak and to the satellite peak in the total current respectively. This figure also shows that the peaks are shifted to higher voltages as \(N_R\) is increased. This shows a strong renormalization of the resonant energies due to the electrodes. In figure 3 we present \(I_{in}^{max}\) vs. \(N_R\) curves for different values of \(N_L\). These curves exhibit a maximum for \(I_{in}^{max}\) as a function of \(N_R\). The optimal configurations correspond to asymmetric structures with wider right barriers. This can be understood by means of the following argument. Increasing the lifetime of the electrons in the well favors the electron-phonon interaction and thus increases the inelastic current. This
Fig. 3. Maximum inelastic current as a function of NR for Nw=20 and Ef=20 meV. can be done by choosing wider (or higher) barriers. In spite of this, as an effect of the asymmetry produced by the applied bias, the lifetime is still controlled mainly by the right barrier. On the other hand increasing the length of the barriers increases the reflectivity of the device diminishing the currents, here it is the left barrier which plays the main role. Then there is a trade off between these two effects that maximizes the phonon emission.

In summary, we have used a simple model to show that the asymmetry in double barrier structures plays an important role in the $I_{in}$-V characteristics and to predict how it can be controlled to optimize LO phonon emission. In particular we show that the optimal configuration corresponds to a collector barrier with a length which doubles that of the emitter.

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Inelastic current $[10^{-8} \text{ A/channel}]$
Maximum inelastic current $[10^{-8} \text{A}]$ as a function of $N_R$ for different values of $N_L$.