Electron-Phonon Effects on Transport in Mesoscopic Heterostructures

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We study the effect of an on-site electron-phonon interaction on the electric transport of mesoscopic heterostructures, described by a tight-binding Hamiltonian with a local electron-phonon interaction. The electronic problem is solved iteratively and the phonon population is found self-consistently. The conductance as a function of the applied bias is calculated using a new formalism suitable to treat many body effects. Double barrier heterostructures are studied. The results compare well with experiments and generalize previous calculations. We also consider a flat potential profile (e.g. a layer of $GaAs$ between a $SiGe$ alloy). The conductance shows an step-wise behavior which is related to the opening of phonon channels when the bias is increased. We propose as well a device which could generate coherent sound.

I. Introduction

The study of electronic transport in mesoscopic heterostructures has created new ideas in the general field of transport in solids which was mainly developed to understand the dynamic of carriers in macroscopic systems. As soon as the size of the system approaches the wavelength of the electron, transport depends upon the interference of propagating electronic waves.

The phonon assisted resonant tunneling in a double barrier heterostructure (DBH), first observed by Goldman, Tsui and Cunnigham[1,2] and studied by several authors[3,4] was an important contribution to the understanding of this problem. The oscillatory behaviour of the conductance in semiconducting point contacts and satellite peaks in double barrier devices are consequences of the electron-phonon interaction.

The theoretical treatment of these systems is rather involved because they are many body systems referring to a far from equilibrium situation, where standard linear response theory does not apply.

Several microscopic models have appeared in the literature to study transport in nanodevices in the presence of electron-phonon interaction. They were treated as a scattering problem which required a two particles Green function[3], as a first order tunneling strength calculation[5] or using the very powerful Keldysh formalism as a nonequilibrium problem[6].

We develop in this paper a formalism capable to treat the many body problem which results from a situation in which electronic carriers interact with phonons as they go through a mesoscopic heterostructure. The problem is treated here within the context of the generalized Landauer-Büttiker formalism[7,8] extended to incorporate the effect of many body interactions. However it is based in a full microscopic model for the electrons, phonons and their interaction, different from the

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trons, phonons and their interaction, different from the phenomenological approach followed by Büttiker to introduce dissipation[9].

In particular we are interested in the case when the distance between the resonant peaks $\Delta\epsilon_P$ approaches the energy of the longitudinal optical (LO) phonon $\hbar\omega_0$. This situation can be easily tailored by controlling the width of the well and the height and width of the barriers. When $\Delta\epsilon_P$ coincides with $\hbar\omega_0$ it is possible to create a situation in which the electrons are injected at the second peak to invert the population. These electrons decay to the lower resonant level emitting coherent LO phonons . This effect, analogous to the laser effect but with sound instead of light could be called SASER and it will be discussed later.

This paper is organized in the following way. In section two we present the model Hamiltonian and also the many body operators adequate to treat it. Section three is devoted to develop the method used to solve the eigenvalue problem introduced in the precedent section and to describe the calculation of the characteristic curve of the system . The fourth section discusses the reliability of the production of coherent ultrasound. Finally in section five are discussed the results for several different physical situations.

II. The model

The system is represented by a nearest neighbors one-dimensional tight- binding Hamiltonian. We neglect the interaction between the electrons and the acoustic phonons because in polar semiconductors like $GaAs$ it is much weaker than the electron optical phonon interaction which is considered in the Fröhlich approximation.

$$\begin{aligned}\mathcal{H} &= \sum_i \epsilon_i c_i^+ c_i \\ &+ t\sum_i (c_i^+ c_{i+1} + c.c.) + \sum_q (\hbar\omega_q) b_q^+ b_q \\ &+ \sum_{iq} g_q e^{iqr_i} c_i^+ c_i (b_q^+ + b_q)\ . \end{aligned} \qquad (1)$$

In this Hamiltonian c_i^+ represent the creation operator of an electron in a state localized at site i with spin σ. The spin index was suppressed to simplify the notation because we do not treat here the magnetic problem. The summation over i includes implicitly a summation over σ. The operator b_q^+ creates a phonon in the well with linear momentum q .The potential profile is included by considering a site dependence of the diagonal matrix elements ϵ_i .

We suppose that at $+\infty$ and $-\infty$ the system is connected with a thermal bath of particles which plays the role of fixing the left and the right Fermi levels ϵ_{F_l} and ϵ_{F_r} .

We are assuming as well that the electron-phonon interaction is restricted to the well whose length L is typically of the order of $10a$ to $50a$ where a is the lattice parameter. In reciprocal space this admits a localization for g_q of the order of $1/L$. Besides, as the coupling g_q is stronger for low q, and for the sake of simplicity we approximate $g_q = g\delta_{q0}$.

The state of the system is expanded in a basis of states $|in>$ which represent an electron localized at site i together with the existence of n phonons in the well.

$$|\psi> = \sum_{in} a_i^n |in>\ . \qquad (2)$$

We assume the basis to be orthonormal such that

$$a_i^n = < in|\psi>\ . \qquad (3)$$

If we define the operators

$$O_i^n = c_i b^n, \qquad (4)$$

we obtain

$$a_i^n = \frac{1}{\sqrt{n!}} < 0|O_i^n|\psi>, \qquad (5)$$

where $|0>$ is the vacuum state.

The equation of motion for these operators can be easily obtained and it writes

$$i\hbar\frac{dO_i^n}{dt} = (\epsilon_i + n\hbar\omega_0)O_i^n + t(O_{i-1}^n + O_{i+1}^n) + gO_i^n(b^+ + b) + ng\sum_j c_j^+ c_j c_i b^{n-1}. \quad (6)$$

The last term in this equation represents an electron-electron interaction mediated by phonons . This is the Migdal term that gives rise to superconductivity . Consistently with neglecting the direct electron-electron interaction we do not consider the one mediated by the phonon field.

We calculate the matrix elements of equation (6) between $< 0|$ and $|\psi >$ and looking for stationary solutions of the problem we obtain the following eigenvalue equations to be solved

$$\hbar\omega\, a_i^n = (\epsilon_i + n\hbar\omega_0)a_i^n + t(a_{i-1}^n + a_{i+1}^n) + g(\sqrt{n+1}\, a_i^{n+1} + \sqrt{n}\, a_i^{n-1}) . \quad (7)$$

III. The calculation

As illustrated in Fig. 1, $i = 0$ is the first site of the DBH left barrier. For $i < 0$ we have $\epsilon_i = 0$ and we can consider $g = 0$. Therefore the system (7) decouple into a set of independent equations that can be solved analytically. The solution is

$$a_i^n = I_n e^{ik_n x_i} + R_n e^{-ik_n x_i}, \qquad i < 0, \quad (8)$$

where k_n is defined by the dispersion relation

$$\hbar\omega = n\hbar\omega_0 + 2t\cos k_n a, \quad (9)$$

where $t < 0$.

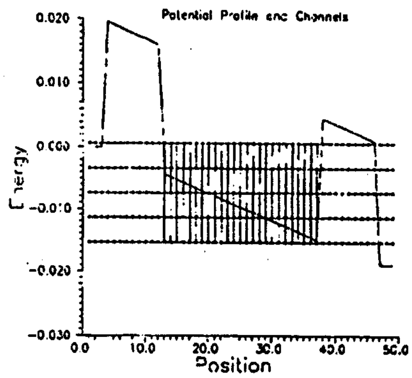

Figure 1: It is shown the potential profile for an applied bias $V = 0.02t$. The position is measured in units of the lattice parameter. For this situation five channels are possible.

For a real k_n the first term in equation (8) represents an incident wave and the second a reflected one.

It is convenient to define the energy measured from the bottom of the conduction band $\epsilon \equiv \hbar\omega - 2t$

$$\epsilon = n\hbar\omega_0 + 2t(\cos k_n a - 1). \quad (10)$$

The second term in equation (10) is the kinetic energy of the electron. For n greater than some n_0 this kinetic energy turns out to be negative (n_0 is zero if the Fermi energy ϵ_F is less than the LO phonon energy $\hbar\omega_0$ as it is usual). That means that we have $k_n = i\kappa_n$ and the solutions take the form

$$a_i^n = I_n e^{-\kappa_n x_i} + R_n e^{\kappa_n x_i}, \qquad i < 0. \quad (11)$$

In this case the amplitudes I^n have to be zero for these modes in order to assure a regular behavior for $x \to -\infty$. They are vanishing modes at left.

On the other hand for $i > N$ we have a flat potential profile, i.e. $\epsilon_i = -V$ where V is the applied bias, and as $g = 0$ in this region as well, the system of equations is decoupled.

Without lose of generality we can assume that there are no incoming waves from the right. The solution can be written then as

$$a_i^n = T_n e^{ik'_n x_i}, \qquad i > N \quad (12)$$

where k'_n fulfill the dispersion relation

$$\hbar\omega = -V + n\hbar\omega_0 + 2t\cos k'_n a. \quad (13)$$

We have not solutions with negative kinetic energy at the right part of the system.

The problem reduces now to make compatible the left with the right solutions what can be easily achieved by numerically iterating equation (7). The process is very fast and yields the exact solution of this model.

From equation (7) we can get the coefficients at site $i-1$ as explicit functions of the two following sites.

$$\begin{aligned} a_i^{n-1} &= [(\hbar\omega - \epsilon_i - n\hbar\omega_0)/t]a_i^n \\ &- (g/t)(\sqrt{n+1}\, a_i^{n+1} + \sqrt{n}\, a_i^{n-1}) - a_{i+}^n (14) \end{aligned}$$

We calculate from expression (12) the coefficients at two consecutive sites with $i > N$ as a starting point. By choosing $T_n = 0$ for some channel and zero for the others and iterating (14) we get the expansion coefficients a_i^n at two successive sites with $i < 0$ from which the incident and reflected waves amplitudes can be calculated. This correspond to arbitraries values for I_n and R_n, and in general I_n will not be zero for the channels below the conduction band. Therefore these solutions have no physical meaning. However, as the relation between input (left) and output (right) is linear, we can calculate the response $T_{n(l)}$, $R_{n(l)}$ for an arbitrary input I_n .

Let us define matrices $\mathbf{M_T}$ and $\mathbf{M_R}$ such that

$$T_{n(l)} = \sum_m M_{Tmn} I_{n(l)} \quad (15)$$

$$R_{n(l)} = \sum_m M_{Rmn} I_{n(l)} \quad (16)$$

or, shortly $\mathbf{T} = \mathbf{M_T I}$, $\mathbf{R} = \mathbf{M_R I}$

As we start from the right we have to express $\mathbf{I}$ and $\mathbf{R}$ as functions of $\mathbf{T}$ by inverting the former relations

$$\mathbf{I^0} = \mathbf{M_T^{-1} T} = \mathbf{G_I T} \quad (17)$$

$$\mathbf{R^0} = \mathbf{M_R M_T^{-1} T} = \mathbf{G_R T} \quad (18)$$

For the sake of simplicity we start with $T_{n(l)} = \delta_{nl}$ and then from the amplitudes calculated iteratively we get $\mathbf{G_I} = \mathbf{I^0}$ and $\mathbf{G_R} = \mathbf{R^0}$. After that it is straightforward to obtain $\mathbf{M_T} = \mathbf{G_I^{-1}}$ and $\mathbf{M_R} = \mathbf{G_R G_I^{-1}}$.

As it was discussed above, the situation for $\epsilon_F \leq \hbar\omega_0$ corresponds to $I_n = I_0\delta_{n0}$ that yields the result

$$T_n = (G_I^{-1})_{n0} I_0 \quad (19)$$

$$R_n = (G_R G_I^{-1})_{n0} I_0 \quad (20)$$

and gives the response to an incoming electron with energy $0 \leq \epsilon \leq \epsilon_F$.

Our purpose is to calculate the characteristic curve of this device. This can be achieved calculating directly the current J.

In the region outside the well in which $g = 0$ the system decouples into independent channels and the current is easily calculated . From the Hamiltonian (1) we obtain the continuity equation

$$\frac{dQ_i}{dt} + (J_{i+1/2} - J_{i-1/2}) = 0 \quad (21)$$

where $Q_i = e c_i^+ c_i$ is the charge operator at site i and $J_{i+1/2}$, the current operator at the bond linking sites i an $i+1$, is defined as

$$J_{i+1/2} = (et/\hbar i)(c_i^+ c_{i+1} - c_{i+1}^+ c_i) \quad (22)$$

from which we get the average current at this place

$$j_{i+1/2} \equiv <\psi|J_{i+1/2}|\psi> = (2et/\hbar)\sum_n \mathcal{I}m(a_{i+1}^{n*} a_i^n) \quad (23)$$

For $i > N$, a_i^n has the simple analytical expression (12) and we get

$$j_{i+1/2} = (2et/\hbar)\sum_n |T_n|^2 \sin k'_n a, \quad (24)$$

and each term (i.e. the current in each channel) is site independent as expected. In the same way for $i < 0$ we get

$$j_{i+1/2} = (2et/\hbar) \sum_{n \leq n_0} (|I_n|^2 - |R_n|^2) \sin k_n a, \quad (25)$$

It can be seen that the current is conserved in our model.

For the case $\epsilon_F \leq \hbar\omega_0$ this expression reduces to

$$j_{i+1/2} = (2et/\hbar)(|I_0|^2 - |R_0|^2) \sin k_0 a, \quad (26)$$

because $n_0 = 0$

In order to get the total current we have to sum over all the states below the Fermi energy. This sum is transformed in an integral over energies and taking into account that for the zero channel at left, $\rho(\epsilon) = \sin^{-1} k_0 a$ we get the simple expression

$$j_T = (4et/\hbar) \int_0^{\epsilon_F} (|I_0|^2 - |R_0|^2) d\epsilon, \quad (27)$$

where we have assumed one incoming electron per state k_0 and spin.

IV. Coherent sound

The formalism developed here by contrast with the one described by Ref. [4] is not limited to treat the situation in which $\Delta\epsilon_P \gg \hbar\omega_0$. This limitation arise there from the reduction of the well to a single point via a renormalization. Besides, our formalism permits to treat the phonon system coupled with electrons traversing the well.

The device proposed here consist in a double barrier system with a wide well in between in such a way that the energy difference $\Delta\epsilon_P$ between the first and the second peak localized within it, coincides with the phonon energy. The energy $\Delta\epsilon_P$ depends upon the applied potential because the well becomes approximately triangular with an inclination determined by the bias. If the barriers are wide or high the width of the resonant peaks diminishes and its spontaneous half-life increases. The width of the well and the barriers can be easily controlled in samples grown by molecular beam epitaxy. For $GaAs-GaAlAs$ samples, the height of the barriers can be also controlled through the aluminum concentration.

If the half-life of the electrons traversing the well with energy corresponding to the first excited peak is long enough, the population in the well is inverted (as it occurs in diode laser). When an electron relaxes by emitting a LO phonon, this elastic excitation is confined to the well[10,11]. The presence of this vibration at a frequency that coincides with $\Delta\epsilon_P$ will stimulate the emission of new phonons in phase with the first one. It can be seen in our Hamiltonian that the probability of stimulated emission is equal to the probability of absorption. As the population is inverted the process continues, producing a great number of coherent phonons, until the heat produced by the decay of LO phonons (and by electrons also) put the system out of the resonance condition. The system can be pumped continuously by injecting electron but probably it will be necessary to work in a pulsed regime.

Several shortcomings have to be overcome in order to produce this device in a laboratory. Probably a fine sintony will be required in order to achieve the resonant condition. This can be done through the application of a magnetic field. The continuum due to the free electron motion in the direction parallel to the interface could broaden too much the peaks. This problem could be bypassed by reducing lateral dimensions. Besides, the beam of LO-phonons has a group velocity near zero and they decay by emmiting a pair of acoustic phonon with same energy and opposite wave vectors. The time scale of this decay is a few picoseconds then the beam of LO-phonons is confined close to the well. The secondary beam of acoustic phonons has the half of enenrgy of the primary LO beam and it can propagate outside the device. The beam of acoustic phonons may be no longer coherent. Several other effect could create other difficulties to fabricate the device.

If the coherent ultrasound could be produced, it will have a wide range of applications. As this high frequency sound can propagate through $GaAs$ it will be possible to separate a reference beam and make it to interfere with one that passes through a sample. The registered interference pattern could be used to produce an hologram that reveal the distribution of impurities and defects.

We don't know if very high frequency ultrasound could by used to study biological tissues but, if it were possible, the coherence of the beam will strongly improve the resolution of ecographies and will permit also the production of medical holograms.

V. Results

Here we present the characteristic curves for double barrier heterostructures and for systems with a flat profile.

For $GaAs$ the hopping constant can be taken $t = 5.2eV$ determined from the effective mass $m^* = 0.067$[6]. The LO phonon frequency of bulk $GaAs$ is $\hbar\omega_0 = 36$ meV, an the strength of the electron-phonon interaction is approximately $g = 20$ meV. The other parameters will depend on sample preparation. The height of the barriers varies typically between $40meV \leq e_0 \leq 400meV$ depending on aluminum concentration. The widths of the barriers and the well have a wide range of variation. The Fermi level depends on the doping (n^+) in bulk $GaAs$, and it can be also variate easily . A high Fermi level broaden the peaks.

We have taken a typical symmetric sample composed of a well of 25 layers of $GaAs$ between barriers of 9 layers of $Al_xGa_{1-x}As$. The height of the barriers was taken $e_0 = 100meV$ and the Fermi level at left was set to $\epsilon_{Fl} = 5meV$.

We can observe that the energy difference between the main peak and its satellite $\Delta\epsilon_1$ is not equal to the LO phonon energy $\hbar\omega_0$. This is due to the fact that the potential drop inside the well is less than the applied voltage[5]. As our model assumes a linear variation of the potential due to the applied bias (neglecting the band bending and the asymmetric profile due to nonlinear effects), the potential drop at the middle of the well is half of the applied bias. Therefore we expect a satellite peak for $V = V_p + 2\hbar\omega_0$.

The results are shown in Fig. 2. The applied voltage is measured in units of t. The energy difference $\Delta\epsilon_1 = 43meV$ is very close to the experimental result.

We have also calculated the current for a system with a flat profile. This situation can be achieved experimentally growing layers of $GaAs$ merged in a matrix of a $SiGe$ tailored in such a way that the conduction band offset between them be negligible. The $GaAs-SiGe$ interfaces act as contacts, then the potential drop occurs through the $GaAs$. When the applied voltage increase, new channels are open and the current jumps. In Fig. 3 we can observe these steps. In a real device these discontinuities in the current will be reduced to only discontinuities in the derivaritive of the current due to the motion parallel to the interface.

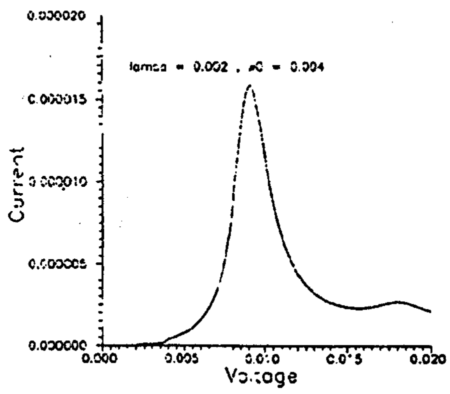

Figure 2: The characteristic curve for a DBH shows the well known satellite peak.

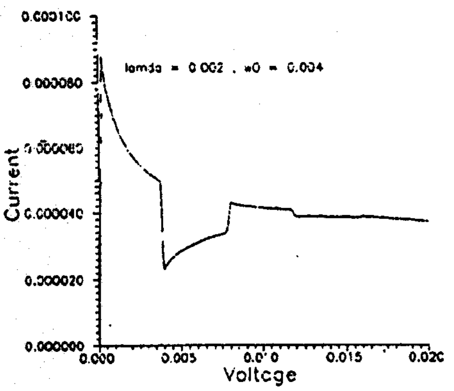

Figure 3: Characteristic curve for a flat profile (see text).

The study of the resonant situation described in the last section requires the inclusion of the half-times of phonons and electrons. LO-phonons can decay in two acoustic phonons and electrons can also relax emitting acoustic phonons. These effects can be included through an imaginary part in the system energy $\hbar\omega \rightarrow \hbar\omega + i\eta$. This calculation is undercourse and it will be published elsewhere.

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