INTRINSIC HIGH FREQUENCY CHARACTERISTICS OF TUNNELING HETEROSTRUCTURE DEVICES

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Abstract

We have developed a general numerical method to solve the periodic time-dependent Schrödinger equation where Quantum Transmitting Boundary Method (QTBM) is used to formulate the boundary conditions of the far-from-equilibrium open systems. The approach is applied to the resonant tunneling diode (RTD) with a superposition of a dc and sufficiently small ac bias. Results of the linear admittance, rectification coefficient and second harmonic generation coefficient are presented as a function of frequency and bias. The calculation has shown that at high frequency (several THz), the intrinsic linear response of RTD becomes capacitive in the NDR region and the rectification coefficient and second harmonic generation coefficient show a resonant enhancement. It indicates that the intrinsic high frequency limit (f_{max}) is influenced more by the electron exchange between the reservoir and the resonant state in the well than by the resonant width. Our results are consistent with those obtained by Wigner function, but in disagreement with most of the results obtained by Schrödinger equation and Green's function. This contradiction is solely due to the problems of definition of reactive current component in the literature.

I INTRODUCTION

High speed device and circuit applications generate considerable interest for the study of the tunneling heterostructure devices. Since the first detection of resonant tunneling diode (RTD) at 2.5 GHz by Sollner and co-workers [1] both experimental and theoretical research work have been widely carried out [2-6].

The existing theoretical results unfortunately conflict with one another. For example, those obtained by conventional tunneling theory based on Schrödinger equation predict inductive behavior at high frequency while Wigner function gives capacitive results. To settle the contradiction, we have developed a systematical numerical method based on single-particle Schrödinger equation with boundary conditions set up by Quantum Transmitting Boundary Method (QTBM)[7]. This method performs task under any bias condition. The application to RTD shows a consistent characteristics with that of Wigner function. The electron exchange between the reservoir and the resonant state in the well plays more important role in the high frequency response than we expected. Two definitions of the current reactive component are to be discussed and compared, which will unify the conflicting results by different approaches.

II THEORETICAL MODEL

In this section, an one-dimensional numerical model of periodic time-dependent Schrödinger equation is to be presented. We consider an open system with two boundary regions (reservoirs): left

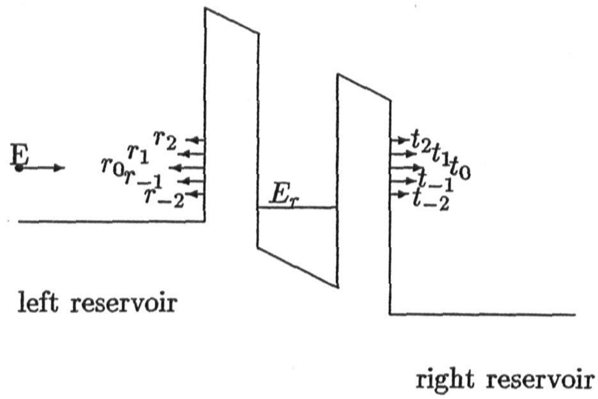

Figure 1: The numerical model of periodic time-dependent Schrödinger equation.

and right. The left voltage is $V_{left} = V_L + \tilde{v}_L \cos\omega t$, the right $V_{right} = V_R + \tilde{v}_R \cos\omega t$, and inside the system $v(x,t) = v_{dc}(x) + \tilde{v}(x)\cos\omega t$. All the incoherent processes are ignored and the flat band potential distribution is assumed, as illustrated in Fig. 1.

Within the open system the wavefunction has the form:

$$\psi(x,t) = \sum_{m=-\infty}^{\infty} \psi_m(x) e^{-im\omega t - i\omega_0 t}. \tag{2.1}$$

Inserting (2.1) into the time dependent Schrödinger equation $i\hbar\partial\psi/\partial t = H\psi$ and collecting terms of equal frequency leads to these equations, in discretized form [8] :

$$\begin{aligned}
-s_j\psi_{0,j-1} + (d_j - E)\,\psi_{0,j} - s_{j+1}\psi_{0,j+1} &= 0,\\
-s_j\psi_{\mp1,j-1} + (d_j - E \pm \hbar\omega)\,\psi_{\mp1,j} - s_{j+1}\psi_{\mp1,j+1} - \left(\frac{\tilde{v}_j}{2}\right)\psi_{0,j} &= 0,\\
&\vdots\\
-s_j\psi_{\mp m,j-1} + (d_j - E \pm m\hbar\omega)\,\psi_{\mp m,j} - s_{j+1}\psi_{\mp m,j+1} - \left(\frac{\tilde{v}_j}{2}\right)\psi_{\mp(m-1),j} &= 0,
\end{aligned} \tag{2.2}$$

where d_j and s_j are the diagonal and off-diagonal elements of the Hamiltonian matrix defined in [8], respectively.

Since we are now dealing with the open system, the appropriate boundary conditions should be applied to (2.2). Fig. 1 shows the physical picture of a single electron with energy E incident from the left reservoir. At the two boundary regions, the wavefunction can be written as [9] :

$$\psi_B = \sum_{m=-\infty}^{\infty} \left(t_{m,B}e^{ik_{mB}x} + r_{m,B}e^{-ik_{mB}x}\right) e^{-i(\omega_o + m\omega)t} \sum_{l=-\infty}^{\infty} J_l\left(\frac{\tilde{v}_B}{\hbar\omega}\right) e^{-il\omega t}. \tag{2.3}$$

where $B = L$ (left reservoir) or $B = R$ (right reservoir) and $J_l(x)$ is the Bessel function.

We formulate the boundary conditions by implementing Quantum Transmitting Boundary Method (QTBM) to the boundary wavefunctions (2.3). Incorporate these boundary conditions with (2.2), a set of linear equations are readily formed, which compose a block tridiagonal matrix. This final matrix is the system to be solved.

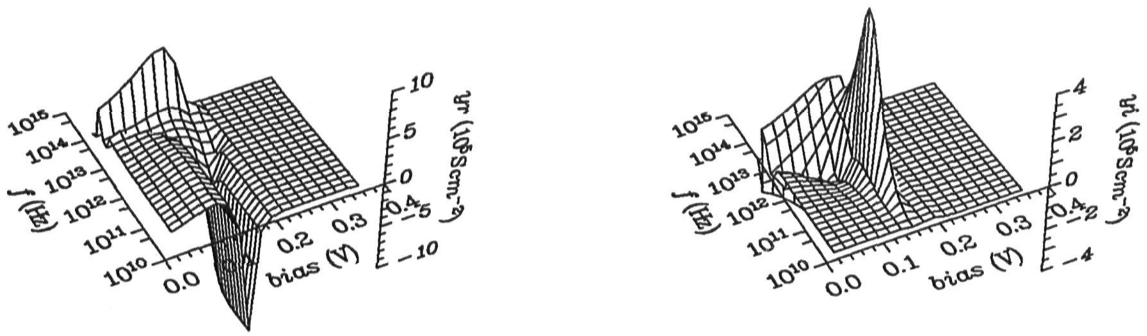

Figure 2: Linear response of a RTD structure.

III AC SMALL SIGNAL RESPONSE

The total current can be represented as:

$$I = -q\hbar/m^* \sum_k P_k Im < \psi^* \frac{\partial \psi}{\partial x} > . \tag{3.1}$$

where P_k is the probability for the wave vector k.

The current components are defined as ($v = \tilde{v}_R - \tilde{v}_L$):

$$I = I_0 + \frac{1}{2}(yve^{i\omega t} + y^* ve^{-i\omega t}) + \frac{1}{4}a_{rect}v^2 + \frac{1}{8}(a_{2\omega}v^2 e^{2i\omega t} + a^*_{2\omega}v^2 e^{-2i\omega t}) \tag{3.2}$$

or one can rewrite the above definition in a sinusoidal form:

$$\begin{aligned} I &= I_0 + Re(y)v\cos(\omega t) - Im(y)v\sin(\omega t) \\ &+\frac{1}{4}a_{rect}v^2 + \frac{1}{4}Re(a_{2\omega})v^2\cos(2\omega t) - \frac{1}{4}Im(a_{2\omega})v^2\sin(2\omega t) \end{aligned} \tag{3.3}$$

Because these authors neglected *the minus sign in the definition of the sinusiodal form*, the inductive results [3,4] claimed by them are essentially capacitive which is in agreement with our calculation as well as with that of Wigner function.

IV RESULTS

We apply our method to a GaAs/AlGaAs RTD structure with barrier width 28.25 A and well width 45.2 A. The results of the linear response ($yr = Re(y)$, $yi = Im(y)$) and the nonlinear reponse of the second order($a_{2\omega}$, a_{rect}) are demonstrated in Fig. 2 and Fig. 3. Our calculations confirm that the linear response of RTD is capacitive at high frequencies and the nonlinear responses ($a_{2\omega}$ and a_{rect}) do show enhancement peaks. According to our calculation the f_{max} derived from the linear responses and the peak positions of the nonlinear responses are less influenced by the width of the resonant state E_r. They are more closely related with the energy difference between the resonant state E_r and the reservoir.

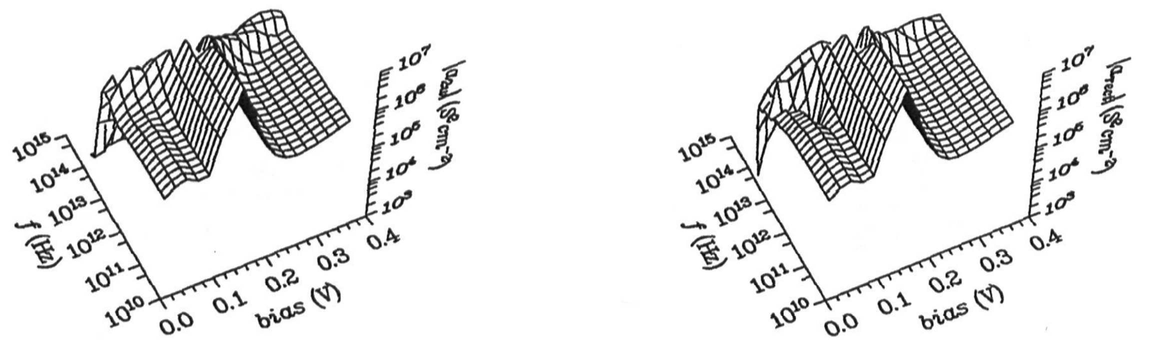

Figure 3: Non-linear response of a RTD structure.

V CONCLUSIONS

We have demonstrated for the first time the three dimensional plots of the linear admittance and the nonlinear responses of the second order for a RTD structure as a function of bias and frequency. The results obtained from the periodic-time dependent Schrödinger equation and Wigner function are characteristically agreeable. The numerical method presented here is able to be applied to any tunneling heterostructure with arbitrary potential distribution within the device.

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