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Density of Electronic States in a Biased Resonant Tunneling Structure

by

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Density of Electronic States in a Biased Resonant Tunneling Structure

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Abstract

We calculate the change in the density of states due to a biased resonant tunneling structure. The maximum of the density of states near resonance gets shifted towards low-energy side compared to the unbiased case, as is the transmission coefficient, although the two need not be identical. For the case of asymmetric barrier heights, the left-right symmetry of the density of states is broken when the field is non-vanishing.

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In recent years scientists have become increasingly aware of the importance of resonant tunneling structures (RTSs) in electronic and opto-electronic device applications and their possible role in fundamental advances.[1-5] Therefore, many studies of static and dynamic aspects of resonant tunneling structures have been undertaken. A common static quantity of interest is the transmission coefficient $T(E)$; a related physical quantity is the width of the resonance peak, which is inversely proportional to the lifetime of the resonant state. A second important static quantity is the density of states, a knowledge of which is essential in understanding transition probabilities, dielectric functions and absorption and luminescence characteristics.

Recently the local density of states,

$$N(E,x) = \sum_n \delta(E-E_n) \, |\psi_n(x)|^2 \quad , \tag{1}$$

in a RTS has been obtained and analyzed in various limits.[6,7] Here E_n are the energy eigenvalues of the system and ψ_n are the corresponding eigenstates. The global density of states obtained by integrating Eq. (1) following Ref. 6 would be identically zero. We therefore follow a different scheme to calculate the global density of states,[8]

$$N(E) = \sum_n \delta(E-E_n) \quad . \tag{2}$$

In a big box of size L ($L \rightarrow \infty$), the energy levels form a quasi-continuous spectrum. Introduction of a structure inside the box changes the spacing between the levels and produces a change $\Delta N(E)$ in the global density of states, which we calculate. In the neighborhood of a resonance, the changes in the spacing of the energy levels produces a pronounced change in density of states. If the resonances are sufficiently narrow, $\Delta N(E)$ and $T(E)$ coincide; however, for broad resonances this is not true.

For the sake of completeness, we briefly review our method for obtaining the density of states $\Delta N(E)$ for an unbiased RTS.[8] For a flat box extending from $x = 0$ to $x = L$, the density of states in k-space is $N_0(k) = L/\pi$, where $E = \hbar^2 k^2/(2m^*)$ is the energy and m^* the effective mass. Suppose now that the RTS is placed in the middle of the box, at $x = x_1 = L/2$, thereby squeezing more states into some energy region and depleting states in some other region. Suppose that the energy eigenvalues of the system are obtained from the condition $D(k) = 0$ where $D(k)$ is a determinental function of the solutions to the Schrödinger equation (see Eq. (9) below). The change in density of states associated with the n-th level having spacing Δk_n is

$$\Delta N(k_n) = \left(\frac{1}{\Delta k_n} - \frac{L}{\pi}\right) . \tag{3}$$

The spacing Δk_n is easily obtained by finding the roots of the eigenvalue condition $D(k) = 0$ with the use of a Newton-Raphson method or any other appropriate scheme. As the previous work in our group emphasized,[8] the shifts of the energy levels depend sensitively on the phase of the wave function at the position where the structure is introduced (i.e., at $x_1 = L/2$ in this case). This phase dependence produces apparently irregular spacings of the levels, and one has to calculate two "sub-densities" (since the RTS is in the middle) in the manner indicated above and add the two to obtain the total density. As expected, for a biased RTS, calculation of $\Delta N(k)$ and hence $\Delta N(E)$

is more complicated, and the phase of the wave function in the neighborhood of the structure has to be constantly adjusted (by changing the position x_1 to $x_1'(E)$) to get the sub-densities correctly. The position x_1' at which the biased RTS should be placed is obtained from the relation

$$k'x_1' = kx_1 \quad , \tag{4}$$

where $k = (2m^*E/\hbar^2)^{\frac{1}{2}}$, $x_1 = L/2$ and $k' = [2m^*(E+V_o)/\hbar^2]^{\frac{1}{2}}$. Here V_o is the potential drop across the double barrier structure and is taken to be 10 meV throughout this work.

In Fig. 1 we show the geometry of the device. The RTS has an extension $x_3 = a_1 + a_2 + d$, where a_1 and a_2 are the barrier widths and d is the well width. The barrier heights are taken to be V_1 and V_2. The electric field in the structure is uniform and is $F = V_o/x_3$. The electric potential at any point x inside the structure is

$$V_F(x) = V_o(x_1-x)/x_3 \quad . \tag{5}$$

We label the regions of piecewise continuous potential profiles by integers, from 0 to 4, as indicated in the figure, and solve the stationary-state Schrödinger equation for the envelope function in the effective mass approximation where we assume, for simplicity, the same $m^* = 0.067\ m_e$ (m_e = electron mass) throughout the structure. In region 1, for example, the Schrödinger equation is

$$d^2\psi/dx^2 - (2m^*/\hbar^2)[V_F(x) + (V_1-E)]\ \psi(x) = 0 \quad . \tag{6}$$

This can be reduced to

$$d^2\psi(\rho)/d\rho^2 - \rho\psi(\rho) = 0 \quad , \tag{7}$$

whose solutions are the Airy functions, $A_i[\rho(x)]$, and the complementary Airy functions $B_i[\rho(x)]$,

$$\psi(\rho) = A_1 A_i(\rho) + B_1 B_i(\rho) \quad , \tag{8}$$

where A_1 and B_1 are two arbitrary constants, $\rho(x) = \alpha[(x_1 - x) + (V_1 - E)x_3/V_o]$ and $\alpha = [2m^*V_o/(\hbar^2 x_3)]^{1/3}$. The solutions in all the five regions can be obtained in a similar fashion. The eigenvalue condition is the condition of the vanishing of the wave function at x = L, so that

$$D(k) = A_4 \sin k'(L - x_2) + B_4 \cos k'(L - x_2) = 0 \quad , \tag{9}$$

where $x_2 = x_1 + x_3$, and A_4 and B_4 are obtained by demanding the usual continuity of the wave function and its first derivative with respect to x across the interfaces:

$$[A_4 \ \ B_4]^t = \hat{M}\ [\sin kx_1 \ \ k\cos kx_1]^t \tag{10}$$

The 2 x 2 matrix $\hat{M}$ in the equation above is

$$\hat{M} = \hat{M}_{34}^{-1}(R)\hat{M}_{34}(L)\hat{M}_{23}^{-1}(R)\hat{M}_{23}(L)\hat{M}_{12}^{-1}(R)\hat{M}_{12}(L)\hat{M}_{01}^{-1}(R) \quad . \tag{11}$$

The subscripts on the matrices indicate the two regions they connect, and L and R stand, respectively, for the left and right sides of the interface.

Equations (3), (4), (10) and (11) enable us to obtain $\Delta N(E)$ for a biased RTS, which can then be compared with the transmission coefficient T(E) obtained in the usual way. We call the structure shown in Fig. 1 as a tilted box with a structure (TBWS). We define a background potential profile called the tilted box (TB) for which $V_1 = V_2 = 0$ in Fig. 1. The difference in density of states between TBWS and TB gives $\Delta N(E)$, which can be compared directly with T(E).

Figures 2-4 show T(E) and $\Delta N(E)$ for a double barrier device of barrier widths 50 Å each and heights 200 meV each, and a well width of 100 Å. Figures 2 and 3 show T(E) and $\Delta N(E)$ for the first two bound state resonances, whereas Fig. 4 is for energies above the barrier energy. A comparison with the unbiased case shows that both T(E) and $\Delta N(E)$ get shifted to lower energies than the corresponding unbiased case.

For the sake of completeness, we comment on the physical origin of the energy shift of transmission resonances due to the electric field. The electron resonance energy is a compromise between the increased kinetic energy due to a spatially-varying potential and the lowering of the potential energy brought about by the field. The electron wave function wiggles a lot to accommodate the increased kinetic energy and lowers its total energy. The electron resonance energy decreases linearly for both the ground state and the first excited state for the electric field considered by us. The magnitude of the rate of decrease with the field is larger for the ground state than the first excited state.

Finally, in Fig. 5 we show our results for an asymmetric double barrier structure without a field ($V_o = 0$) and with a field ($V_o = 10$ meV). The dot-dashed curves in Fig. (7a) and (7c) represent the field-free case, and these have left-right symmetry with respect to the interchange of the two barriers. In the presence of a field, this symmetry is broken. The dashed lines correspond to the case $V_1 = 100$ meV and $V_2 = 200$ meV, whereas the dotted line corresponds to the permuted case $V_1 = 200$ meV and $V_2 = 100$ meV. This asymmetry is important in calculating tunneling currents and transition probabilities.

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Figure Captions

1. metry of the tilted box with a structure (TBWS). The box extends from $x = 0$ to $x = L$ (we take L to be of the order of 1.5×10^6 Å to 1.0×10^6 Å in this work) whereas the structure extends from $x = x_1$ to $x = x_1 + x_3$, where $x_3 = a_1 + a_2 + d$. The external electric field is $F = V_o/x_3$. We take $V_o = 10$ meV throughout this paper. The zero of the energy for this and the following figures (Figs. 2-5) is taken to be the bottom of the left-most part of the box.

2. Transmission coefficient T(E) and density of states ΔN(E) for a symmetric double barrier structure (DBS) in an applied electric field. The barriers are each 50 Å wide and 200 meV high, and the well is 100 Å wide. The energy range shown is in the neighborhood of the first resonance energy. The middle panel shows ΔN(E) for a tilted box (TB), (solid curve) and a TBWS (dashed curve).

3. T(E) and ΔN(E) as in Fig. 2, but for the second resonant state.

4. T(E) and ΔN(E) as in Fig. 2, but for the energies above the barrier energy.

5. Transmission coefficient T(E) and density of states ΔN(E) for an asymmetric DBS. The barriers and the well are each 50 Å wide, and the barrier heights are 100 meV and 200 meV. The dash-dotted curves show T(E) and ΔN(E) without the field, and these curves exhibit left and right degeneracies. The dotted curves are for $V_1 = 200$ meV and $V_2 = 100$ meV, whereas the dashed curves are for $V_1 = 100$ meV and $V_2 = 200$ meV. The solid curve in the middle panel is for a tilted box, as explained in the caption to Fig. 2.

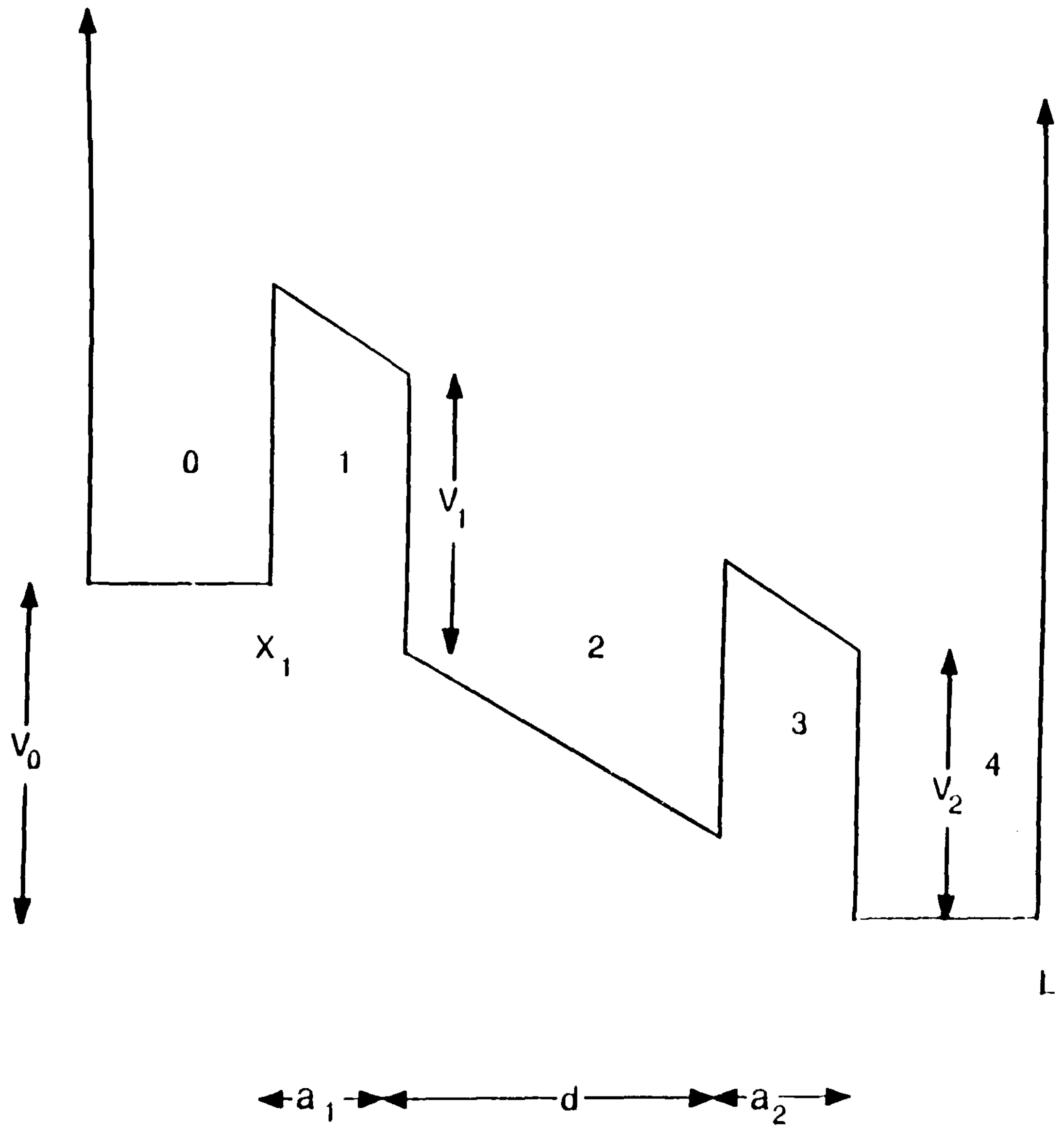
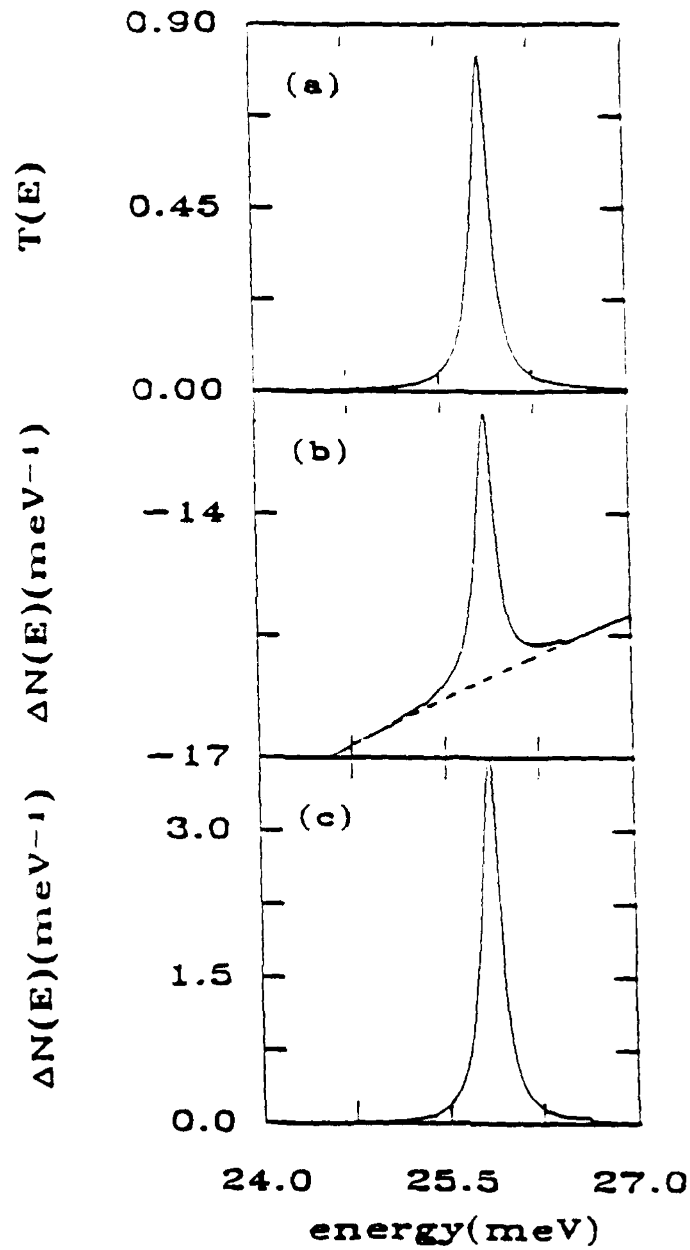


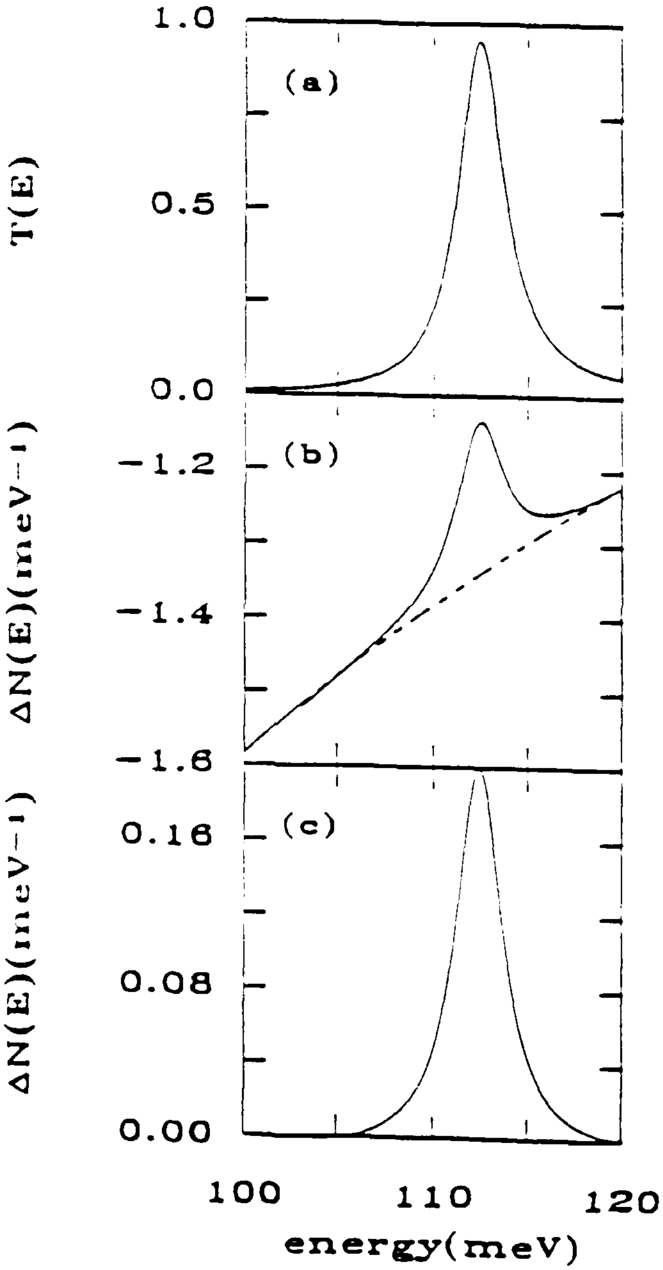
Fig. 1

Fig. 2



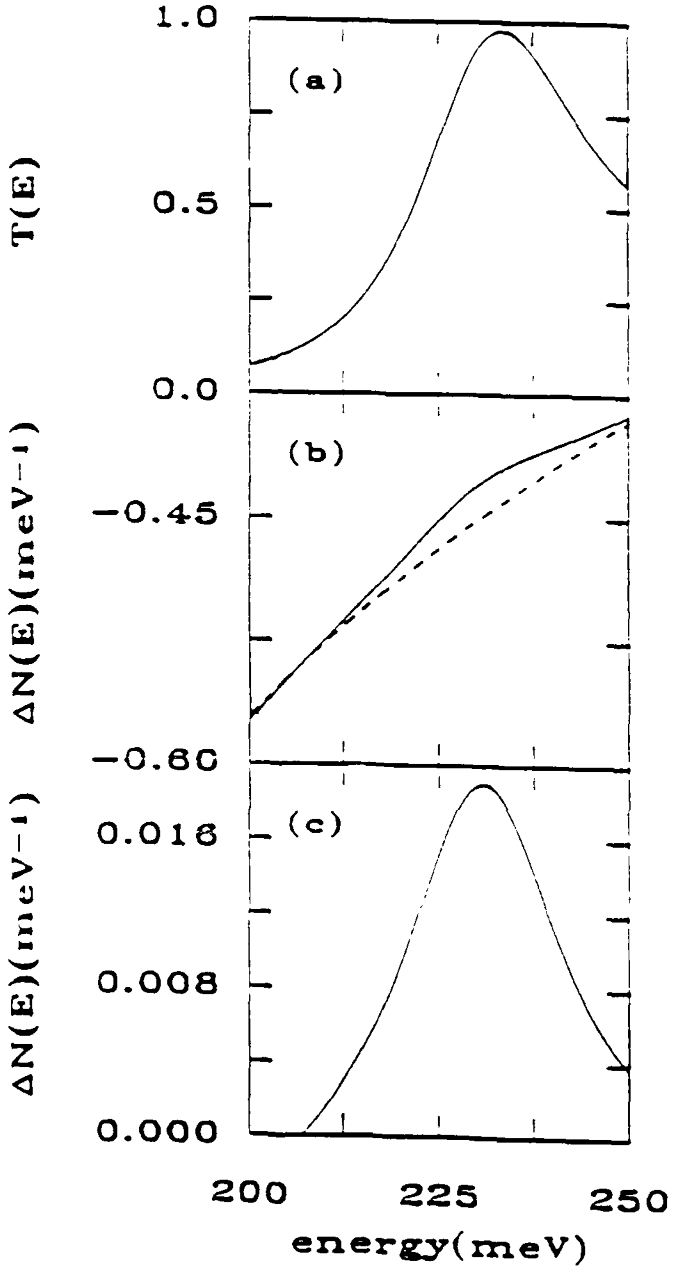
0.90
0.45
0.00
T(E)
(a)
(b)
-14
-17
ΔN(E)(meV-1)
(c)
3.0
1.5
0.0
ΔN(E)(meV-1)
24.0
25.5
27.0
energy(meV)

Fig. 3



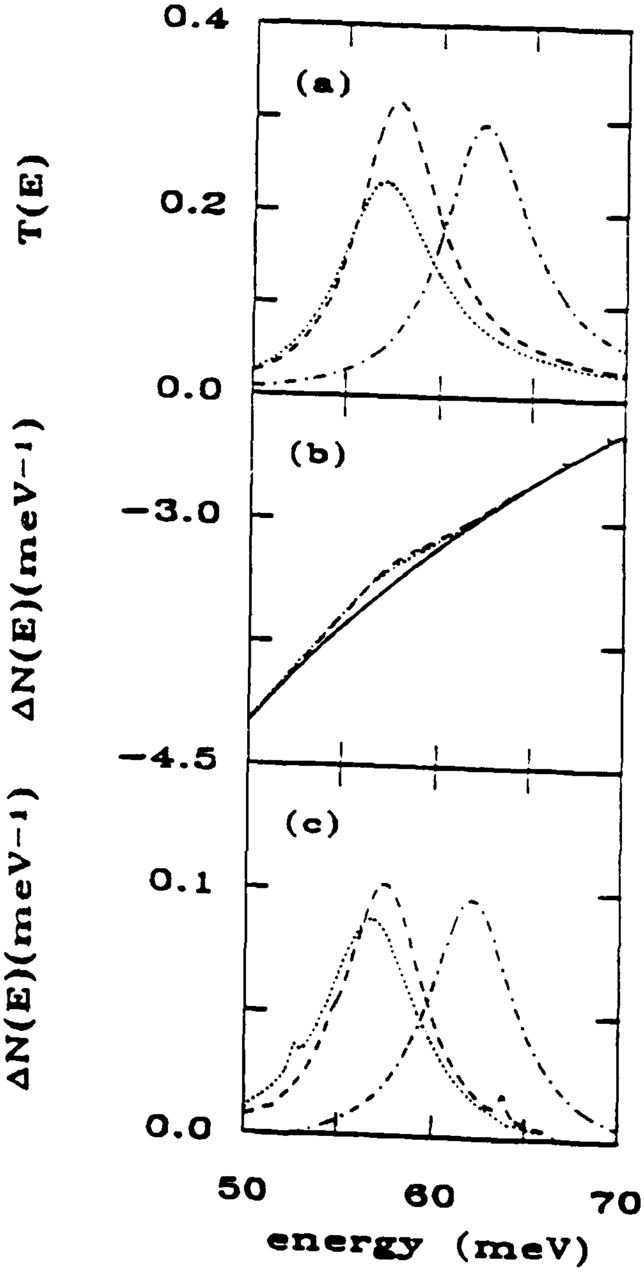
1.0
0.5
0.0
T(E)
(a)
-1.2
-1.4
-1.6
ΔN(E)(meV⁻¹)
(b)
0.16
0.08
0.00
ΔN(E)(meV⁻¹)
(c)
100
110
120
energy(meV)

Fig. 4



1.0
0.5
0.0
T(E)
(a)
(b)
−0.45
−0.60
ΔN(E)(meV−1)
(c)
0.016
0.008
0.000
ΔN(E)(meV−1)
200
225
250
energy(meV)

Fig. 5



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