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LETTER TO THE EDITOR

Elastic and inelastic resonant tunnelling in narrow-band systems: application to transport in minibands of semiconductor superlattices

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Abstract. We consider tunnelling in systems with a finite conduction bandwidth. A physical realization of such a system would be a disrupted semiconductor superlattice imbedded in the base of a n–p–n transistor. There it is possible to tune the energy of the incoming injected carriers by changing the emitter to base voltage. Hence the calculated transmission coefficient, weighted with the energy distribution of the injected electrons, bears direct relevance to measured I–V characteristics. The vertical transport in the unperturbed miniband is described with a tight-binding model, and the disruption, which may arise accidentally, or be fabricated by adjusting the growth conditions, is modelled with an additional double barrier. The transmission coefficient displays a resonant behaviour as a function of energy. Further, we evaluate the transmission coefficient in the case where the region connecting the two superlattices couples to dispersionless optical phonons. Optical-phonon-related satellite features are identified. Finally, the relation of the calculated effects to recent experiments is analysed.

Resonant tunnelling in semiconductor heterostructures is currently a very active area of research. It is becoming increasingly clear that for a quantitative comparison between theory and experiment the traditional analysis, based on the pioneering work by Tsu and Esaki [1], is not sufficient because inelastic effects are not accounted for. Inelastic effects manifest themselves in several ways: they are required to produce the accumulation layer on the emitter side of the barrier structure [2, 3], they play a crucial role in determining the bistability of a resonant tunnelling diode [4, 5], and features related to optical phonon interactions have been identified in the experimental I–V curves [6, 7]. In addition to the experimental stimulus, tunnelling in the presence of inelastic processes is a problem of fundamental interest, and not surprisingly many recent theoretical papers have analysed various aspects of these problems [8–12]. In particular, the work reported in [8, 10] shares many common features with the present study. There are some important differences, however. Our emphasis is to include explicitly the effects due to finite bandwidth. The method or Wingreen *et al* [8] is analytically tractable only in the wide-band limit. Similarly, it is not easy to see how the calculational scheme of Cai *et al* [10] could be modified to take into account a finite bandwidth. In addition, this scheme is perturbative (in the phonon coupling)

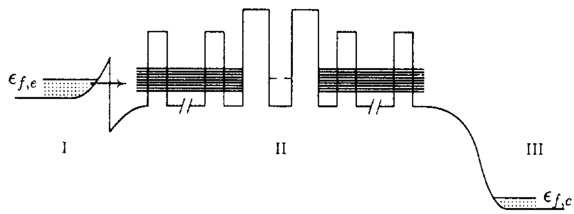

Figure 1. A model of a disrupted superlattice placed in the base of a n–p–n bipolar transistor [15]. By changing the emitter (region I) to base (region II) voltage, electrons can be injected at different energies in the miniband (indicated by parallel lines). The disruption in the superlattice, modelled by a double barrier, supports one quasibound state, indicated by the broken line. Resonant tunnelling through the disruption occurs when the energy of the injected electron matches the energy of the quasibound state.

while the method due to Gelfand *et al* [9], which is employed in the present work, can easily be evaluated to any desired numerical accuracy.

In this letter we study a new resonant tunnelling system, and inelastic effects therein: a superlattice with a disruption. The superlattice is placed in the base of a transistor with a ballistic launcher in a structure similar to the ones proposed by Capasso and Kiehl [13]. The experimental situation we envisage is shown in figure 1. The disruption may be caused by either some uncontrollable agent, or by intentionally modifying the growth conditions. The following observations have motivated our study. First, coherent transport in a miniband has recently been demonstrated [14, 15]. Secondly, Gelfand *et al* [9] have recently developed a theoretical framework for inelastic tunnelling through a *single barrier* within a tight-binding model, where the energy–momentum relation is $E(p) = -2t\cos(pa)$. We suggest that this model has direct physical relevance to transport in a miniband formed in a superlattice: the parameter t is the overlap integral, and in principle it can be obtained from the superlattice parameters, and a is the superlattice periodicity. Further, we interpret the parameter V_0, which Gelfand *et al* [9] view as the height of a tunnelling barrier, as resulting from a disruption in the superlattice, which leads to either a modified site energy, or differing overlap integral(s). A single barrier, however, leads to a smooth behaviour in the transmission coefficient; much more dramatic behaviour is found for the double barrier considered in this work. We can use the formalism of Gelfand *et al* [9] directly: the only generalization required is to use propagators for a double barrier (rather than a single barrier), see below.

The formalism has been described adequately in the original work by Gelfand *et al* [9] and here we summarize only the features specific to our work. The Hamiltonian we consider is $H_{ij} = H^0_{ij} + H^1_{ij}(t)$, where the static part models the disrupted superlattice, and the time-dependent part is the electron–phonon interaction. Explicitly, they are given by

$$H^0_{ij} = -t_{ij} + V_0\delta_{ij}(\delta_{i,-1} + \delta_{i,+1}) \tag{1a}$$

$$H^1_{ij} = V_1\delta_{ij}\delta_{i0}(b\,\exp(-\mathrm{i}\omega t) + b^\dagger\exp(\mathrm{i}\omega t)). \tag{1b}$$

In writing (1) we made the following simplifying approximations (the detailed derivation of (1) and other related models will be discussed in a forthcoming full paper) which, however, capture the essential physics: (i) the overlap matrix element t_{ij} couples only nearest-neighbour sites; (ii) the barriers are located at sites $i = -1$, and

$i = 1$, respectively; and (iii) the coupling to dispersionless optical phonons is operative at site $i = 0$ [8, 12]. The static transmission coefficient corresponding to H^0 is given by

$$T^0(E) = \frac{1}{|1 - 2V_0/D(\epsilon) - \left(V_0/D(\epsilon)\right)^2 (\mathrm{e}^{2\mathrm{i}\Delta} - 1)|^2} \qquad |\epsilon| \leq 1 \tag{2}$$

where $\Delta = 2pa$, p is the momentum of the incoming plane wave, $\epsilon = E/2t$, and the energy-dependent quantity $D(\epsilon)$ is defined in (4) below. Outside the miniband, i.e. $|\epsilon| > 1$, $T^0(E) = 0$. The information about the double barrier is contained in the Green function $G(i, j; \epsilon)$, and for the present case we need

$$G(j, 0; \epsilon) = \mathcal{H}(j; \epsilon) G(0, 0; \epsilon) \qquad G(0, 0; \epsilon) = \frac{1}{D(\epsilon)} \frac{[D(\epsilon) - V_0(1 - C^2(\epsilon))]^2}{[D(\epsilon) - V_0]^2 - V_0^2 C^4(\epsilon)} \tag{3}$$

where

$$C(\epsilon) = \begin{cases} -\epsilon + \mathrm{i}\sqrt{1 - \epsilon^2} & |\epsilon| < 1 \\ -\epsilon + \mathrm{sgn}(\epsilon)\sqrt{\epsilon^2 - 1} & |\epsilon| > 1 \end{cases} \tag{4a}$$

$$D(\epsilon) = \begin{cases} 2t\mathrm{i}\sqrt{1 - \epsilon^2} & |\epsilon| < 1 \\ 2t\,\mathrm{sgn}(\epsilon)\sqrt{\epsilon^2 - 1} & |\epsilon| > 1 \end{cases} \tag{4b}$$

and

$$\mathcal{H}(j, \epsilon) = \frac{D(\epsilon) C^j(\epsilon)}{D(\epsilon) - V_0(1 - C^2(\epsilon))}. \tag{4c}$$

Following Gelfand *et al* [9], we expand the scattered wave at the origin in multiphonon components,

$$\psi^{\mathrm{s}}(j = 0, t) = \sum_{n=0}^{\infty} (b^\dagger)^n A_n \exp[-\mathrm{i}(E - n\omega)t] + \sum_{n=1}^{\infty} (b)^n B_n \exp[-\mathrm{i}(E + n\omega)t]. \tag{5}$$

The resulting recurrence relations for the operators A_n and B_n are formally identical to the ones derived by Gelfand *et al* [9], with (3)–(4) replacing their Green function, and are solved in a similar fashion. The details of the solution are deferred to a future publication; here we only want to point out that in order to obtain numerical convergence virtual processes of fairly high order (fifth order for the present parameter values) must be included. This suggests that caution must be exercised when employing straightforward perturbation theory.

The transmitted current can be evaluated from $\psi^{\mathrm{s}}(0)$ for the present three-site problem with the result

$$\begin{aligned} \langle j_{\mathrm{T}} \rangle = {} & 2ta\mathcal{Z}^{-1} \sum_{l=0}^{\infty} \mathrm{e}^{-l\beta\omega} \sum_{n=0}^{\infty}{}' \sqrt{1 - \epsilon_n^2} \left| \mathcal{H}(1; \epsilon_n) \left[\delta_{n0} + \left(\frac{(l+n)!}{l!} \right)^{1/2} \langle l | A_n | l \rangle \right] \right|^2 \\ & + 2ta\mathcal{Z}^{-1} \sum_{l=1}^{\infty} \mathrm{e}^{-l\beta\omega} \sum_{n=1}^{l}{}' \sqrt{1 - \epsilon_{-n}^2} \frac{l!}{(l-n)!} |\mathcal{H}(1; \epsilon_{-n}) \langle l | B_n | l \rangle|^2 \end{aligned} \tag{6}$$

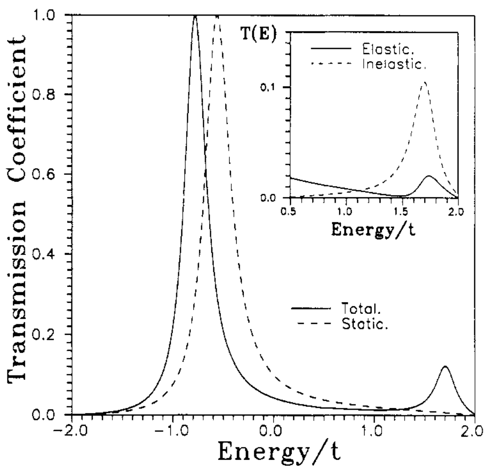

Figure 2. Static transmission coefficient $T^0(E)$ (broken curve) and the total transmission coefficient $T(E)$ (full curve) as a function of the energy in the miniband ($-2t < E < 2t$). The parameters are as follows: $V_0 = 3.0t$, $V_1 = 0.79t$ and $\omega = 2.5t$ at $T = 0$. The inset shows the phonon-related satellite at $E \simeq E_r + \omega$ resolved in its elastic and inelastic components.

where $\epsilon_n \equiv (E - n\omega)/2t$, and the other symbols have the same meaning as in [9]. Comparing with the single-barrier result, the only formal differences are the appearance of the factors $\mathcal{H}(j;\epsilon)$. Finally, the transmission coefficient is given as $T(E) = \langle j_T(E)\rangle/2ta\sqrt{1-\epsilon^2}$.

In figure 2 we show the static transmission coefficient $T^0(E)$, and the total transmission coefficient $T(E)$, resolved into its elastic and inelastic components. The numerical values of the parameters are chosen to mimic experimentally realizable superlattices. We direct attention to the following features. (i) Strong resonance in the transmission coefficient, with a maximum value of unity, both for the static case, and when the phonons are included. The behaviour is in significant contrast to the smooth semi-elliptic behaviour found for the single-barrier case with the maximum value [9] $T_{sb}^{max} = [1 + (V_0/2t)^2]^{-1}$. (ii) Renormalization, or shift, in the main resonance when the phonon interaction is included. (iii) For the chosen parameter values no cusps or singularities are found [9]. (iv) A phonon-mediated satellite peak centred approximately at $E = E_r + \omega$, where E_r is the main resonance energy. This is in accordance with other model studies [8, 10]. (v) The *elastic* component of the total transmission coefficient (contribution proportional to $1 + A_0$ in (6)) displays a phonon echo at $E = E_r + \omega$. This feature is due to virtual-phonon-mediated coupling to the resonant channel. Similar effects in another configuration have recently been reported by Cai *et al* [16].

We now turn to the possible experimental observation of the predicted structure. In a recent experiment [15] a clear negative transconductance (NT) is observed when the superlattice is placed in the base of an n–p–n bipolar transistor. This behaviour can be explained as being caused by conduction through the extended states in a miniband. There is, however, a large background current which may arise for a number of reasons: thermionic emission over the launching barrier, conduction through tail states, or width of the injected electron distribution (both scattering and the range of the incoming energies contribute to this width). It is difficult to separate the effects due to miniband conduction alone, i.e. effects discussed in this work. However, it seems reasonable to assume that the background current is a monotonically increasing function of the emitter to base voltage. If this is the case, the current contribution due to miniband conduction must contain some structure: there are two inflection points in the experimental I–V curve. These would then reflect a similar structure in the miniband transmission coefficients, which is precisely what our calculations indicate. While the above interpretation is only preliminary, we stress that the effects predicted in this paper should be more pronounced if one deliberately fabricates a superlattice with an embedded double barrier.

The simple model described in this letter neglects interactions between the hot carriers in the miniband, and the background cold holes in the p-type base. To estimate these effects the calculation performed by Levi and Yafet [17] should be repeated with the miniband dispersion relation. Further, the transmission coefficient calculated in this work should be averaged over the effective incoming energy distribution. Clearly more work is required before a quantitative comparison can be given.

In summary, we have analysed resonant tunnelling between two sections of a superlattice, and shown that sharp features may arise, with associated phonon satellites. Recent experiments seem to display features which are consistent with those found within our model.

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