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Electron velocity in superlattices

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Abstract. Calculations of the electron velocity in superlattices based on the miniband dispersion relation, and the velocity defined through the tunneling time are discussed. The former definition is based on the intrinsically infinite modified Kronig-Penney model, while the latter rests upon the transfer matrix method and takes the finiteness of the superlattice into account. The main result is that the velocities differ: for weakly coupled structures where the tunneling time can be defined through the linewidth, the transfer matrix method predicts a smaller velocity than the modified Kronig-Penney model.

PACS. 73.21.Cd Superlattices – 73.20.At Surface states, band structure, electron density of states – 73.40.Gk Tunneling – 03.65.Xp Tunneling, traversal time, quantum Zeno dynamics

1 Introduction

In resonant tunneling diodes (RTDs) and short period superlattices (SLs) resonant tunneling dominates the transport behavior [1]. A comprehensive review on superlattice transport was given recently [2]. In the coherent transport regime one important parameter is the transmission coefficient, which is defined as the ratio of the incoming and the transmitted probability current density through the structure. A second important factor is the velocity of electrons inside SLs. The group velocity of the superlattice dispersion relation of the (modified) Kronig-Penney model [3,4] has been widely used in calculations. Here we show that a different velocity definition based upon the tunneling time might be useful in coherent transport. For weakly coupled structures the transmission coefficient has a Lorentzian line shape near the transmission resonances. In these cases the tunneling time of the electrons can be determined from the Half Width at Half Maximum (HWHM) of the resonant peak [5]. From these tunneling times for each individual energy level in a SL, a discrete (non-continuous) velocity – wave vector characteristic can be derived.

2 Comparison between infinite and finite model

The modified Kronig-Penney model assumes an infinite number of superlattice periods. The Bloch condition $\Psi(z+d) = \exp(iqd)\cdot\Psi(z)$ leads to the well known implicit equation [4]:

$$P(E) = \cos(qd), \tag{1a}$$

where

$$P(E) := -\frac{1}{2}\left(\xi + \xi^{-1}\right)\sin k_w w\,\sin k_b b + \cos k_w w\,\cos k_b b,$$
$$\xi = \frac{k_w m_b^*}{k_b m_w^*}. \tag{1b}$$

Here E is the energy, k_w and k_b are the wave vectors in the wells (width w) and in the barriers (width b), respectively, d is SL period, and q is the Bloch wave-vector. For a given (real) q, equation (1b) is only solvable for energies defining the dispersion relation $E(q)$ of the so-called minibands. For one set of material parameters the solution is plotted as the solid line in Figure 1. Due to the time-inversion symmetry of the Hamilton operator of the considered systems the dispersion relation fulfills the condition $E(q) = E(-q)$.

Usually the velocity inside a miniband is then calculated using the group velocity $\nu_g = d\omega/dq$.

The transmission spectra of structures with a finite number of potential periods are generally studied with the help of transfer matrices. For a standard SL with N periods (where each period includes one barrier and one well) the transmission probability is given by [6,7]:

$$T = \left\{1 + \left[\frac{1}{2}\left(\xi - \xi^{-1}\right)\sin k_b b U_{N-1}\big(P(E)\big)\right]^2\right\}^{-1}, \tag{2}$$

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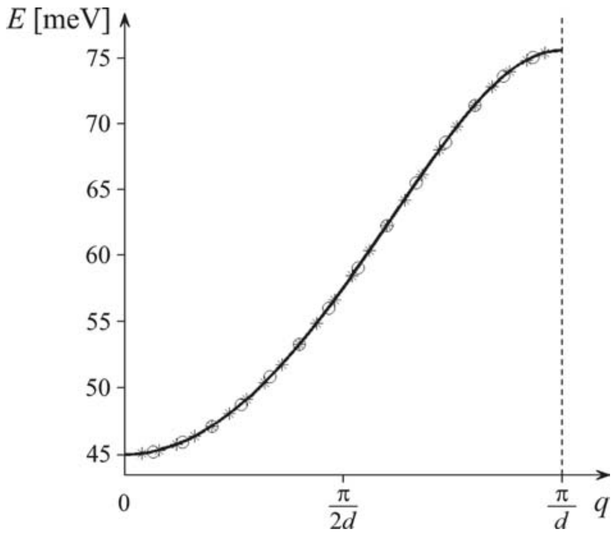

Fig. 1. Dispersion relation for SLs obtained by the modified Kronig-Penney model (solid line – infinite number of potential periods) and by the transfer matrix model (15 (circles) and 25 (asterisk) periods).

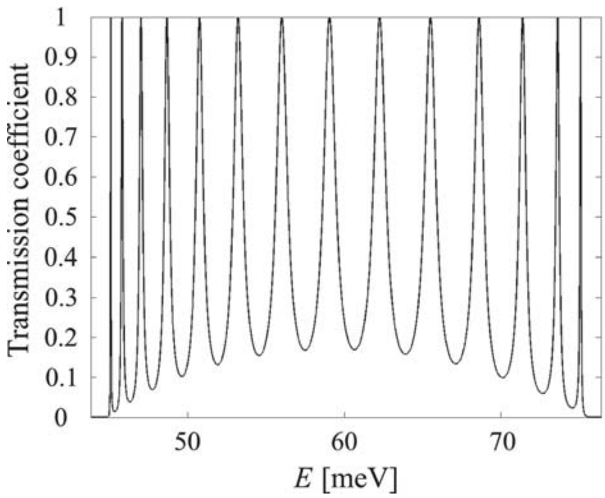

Fig. 2. Transmission spectrum for a GaAs/$Al_{0.3}Ga_{0.7}As$ 6.5/2 nm thick layers semiconductor superlattice with 15 periods, revealing peak positions and widths.

where U_{N-1} denotes the Chebyshev polynomial of the second kind of order $N-1$ and ξ and $P(E)$ have been defined in equation (1b). Recently it was shown [6,8] that the condition for resonances in the SL transmission ($T=1$) is given by:

$$P(E_i) = \cos\frac{i\pi}{N}, \quad i = \pm 1 \ldots \pm (N-1). \tag{3}$$

Identifying the arguments of the cosines in equation (1a) and (3) we end up with the discrete dispersion relation (also shown in Fig. 1, by symbols):

$$P(E_i) = \cos q_i d, \tag{4}$$

where the discrete q_i values are given by [6]:

$$q_i = \frac{i\pi}{Nd} = \frac{i\pi}{L}, \quad i = \pm 1 \ldots \pm (N-1), \tag{5}$$

and $L = Nd$ is the length of the superlattice. Figure 2 shows a typical transmission spectrum (obtained by Eq. (2)) for a SL with 15 periods with characteristic peaks at E_i and corresponding maximum values equal to unity. At these distinct energies the presence of wave functions that spread throughout the whole structure is revealed.

From Figure 2 one can clearly see the different HWHMs, $\Delta E(q_i)$, of the resonant peaks. These resonant tunneling widths implicate the electron lifetime $\tau(q_i)$ in the individual energy levels [5,9]. In the case of 100% transmission probability (and only then!), the electron lifetime $\tau(q_i)$ is equal to the dwell time [10,11] that is a measurable quantity [12,13]. The tunneling time at the resonance energy is also the transition time of a conventional wave-packet [5]. Therefore, it can be used to define the tunneling velocity, $\nu_{tunnel}(q)$, of the finite system:

$$\nu_{tunnel}(q_i > 0) = \frac{L}{\tau(q_i)} = \frac{L \cdot \Delta E(q_i)}{\hbar}, \tag{6}$$

where L is the SL length. In the infinite approach, the electron velocity of a single Bloch state is given by the group velocity [14]. In contrast, in a finite structure the wave function is in general not given by a single Bloch state [8,15]. Consequently the electron velocity (6) can differ from the group velocity.

3 Numerical studies of GaAs/AlGaAs superlattices

We started the study with a SL composed of 6.5 nm thick GaAs wells and 2 nm thick $Al_{0.3}Ga_{0.7}As$ barriers, respectively. We used energy dependent effective masses $m_{b/w} = m_{b/w}(E)$ to account for the non-parabolicity effect [16]. The conduction band offset (barrier height) for these materials is chosen to be 0.28809 eV. (Throughout this work this set of parameters is used.)

3.1 Miniband position

The transmission is essentially zero outside the miniband extending in the range of 44.8 meV $< E <$ 75.6 meV for the first miniband (Fig. 2). The energy levels with their corresponding discrete wave-vectors directly implicate the dispersion relation of the periodic structure. In Figure 1 we compare the discrete dispersion relations for SL with 15 and 25 periods (circles and asterisks), respectively (Eq. (4)), and the continuous one (Eq. (1)). Since a SL with N periods (without additional barrier at the end of the structure) has $N-1$ energy levels in each miniband we see 14 and 24 discrete values, respectively.

Due to the equations (1a) and (4), the discrete values coincide exactly with the continuous ones. The underlying reasons are the same boundary conditions between the interfaces, while only the boundary conditions to the surroundings are different. By increasing the number of SL periods the discrete characteristic looks more and more continuous like matching the modified Kronig-Penney's. Therefore, for higher number of periods it does not matter which model we use to determine the miniband width, while for smaller number of periods, we can make quite rough approximation (in our case deviation of 3% for a 15 period structure).

3.2 Miniband velocity

In Figure 3 we show a comparison between the group velocity and the velocity defined through the tunneling time (tunneling velocity), equation (6), respectively. Like the group velocity ν_g, the tunneling velocity ν_{tunnel} is independent of the SL length since increasing the number of periods increases the length of the SL but decreases the width of the resonances just that much that the velocity stays the same [15]. To confirm this we calculated the maximum tunneling velocity ν_{tunnel} for a SL with 2000 periods. ν_{max} was 9.280×10^4 m/s, and differs slightly from those in Figure 3 for 25 periods (ν_{max} is 9.279×10^4 m/s) only due to the fact that both velocities are not necessarily taken at the same energy and/or due to better approximated peak shape by a Lorentzian for higher number of periods. The most important observation shown in Figure 3 is the big difference between the group velocity and the tunneling velocity ν_{tunnel}. While the shape of both relations is pretty much the same (except at the band edges), the group velocity exhibits a much higher ν_{max} (2.004×10^5 m/s).

To study this discrepancy we calculated both velocity characteristics for an increased barrier width keeping the well width constant (Fig. 4a). Both $\nu(q)$ characteristics change (they both decrease), with the effect of an even bigger difference between them. From these results we can very clearly see the suppression of the electron velocity in all periodic structures, where the energy bands are composed of Lorentzian peaks. If we decrease the barrier width b, the tunneling velocity ν_{tunnel} approaches the group velocity (Fig. 4b) and they become approximately equal for $b = 1.2$ nm. A further decrease of b leads to $\nu_{tunnel} > \nu_g$ (Fig. 4c). The same effect occurs when the barrier width is kept constant and the well width is increased.

To explain these phenomena we studied the transmission spectra. By broadening the barriers and/or the wells the resonant peaks get sharper and more and more Lorentzian – the miniband becomes less coupled (Fig. 4a). In these situations the velocity determined from the HWHM tunneling time is relevant and there is velocity suppression compared to the group velocity. For making

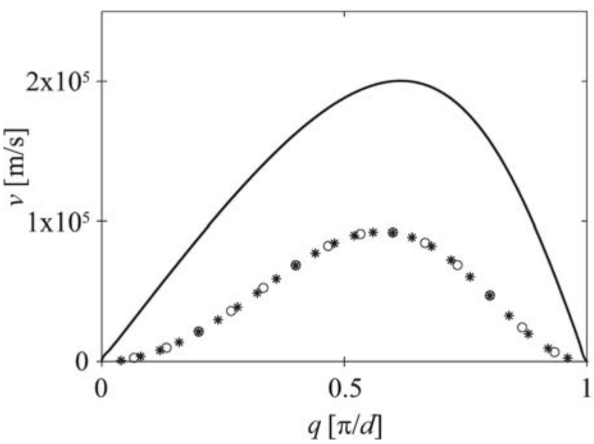

Fig. 3. Group velocity (solid line) and tunneling velocity, equation (6), (discrete values) vs. wave-vector of SLs with barrier width $b = 2$ nm and well width $w = 6.5$ nm. Open circles and asterisks are discrete values for 15 and 25 period SL, respectively. The corresponding transmission spectrum is shown in Figure 2.

the barriers and/or the wells thinner, the coupling increases and the peak shape starts to deviate appreciably from Lorentzian (Fig. 4c). Therefore, the HWHM cannot be used to determine the tunneling time from the transmission spectrum anymore. From a rough estimation we claim that the tunneling velocity approach gives correct results for the velocity in SLs with transmission valley values between the SL resonances below $T = 0.25$. For SLs with non-Lorentzian peaks the velocities cannot be calculated by our model.

4 Discussion

Our explanation for the discrepancy between the group and the tunneling velocity is that both velocity definitions correspond to different physical quantities. The group velocity determines the Bloch electron velocity inside an infinite structure, no matter how the electrons were first inserted. The tunneling velocity takes the injection and extraction of electrons at the boundaries of the SL into account. Our statement that the velocity through finite SLs does not change with the number of periods was based on the observation that the tunneling time increases proportionally to the number of periods. Therefore we can conclude that it is not a constant tunneling time that is additionally spent at the boundaries of the finite SL but that the velocity through the complete structure is suppressed. In order to support this conclusion we modified the outermost barrier widths, b', to influence the coupling between the SL and the surrounding. This modification appreciably changes the transmission spectrum and the tunneling velocity. Figure 5 shows the tunneling velocities for outermost barriers widths of 2.2 and 1.8 nm, respectively, in comparison to a SL where all barriers are the

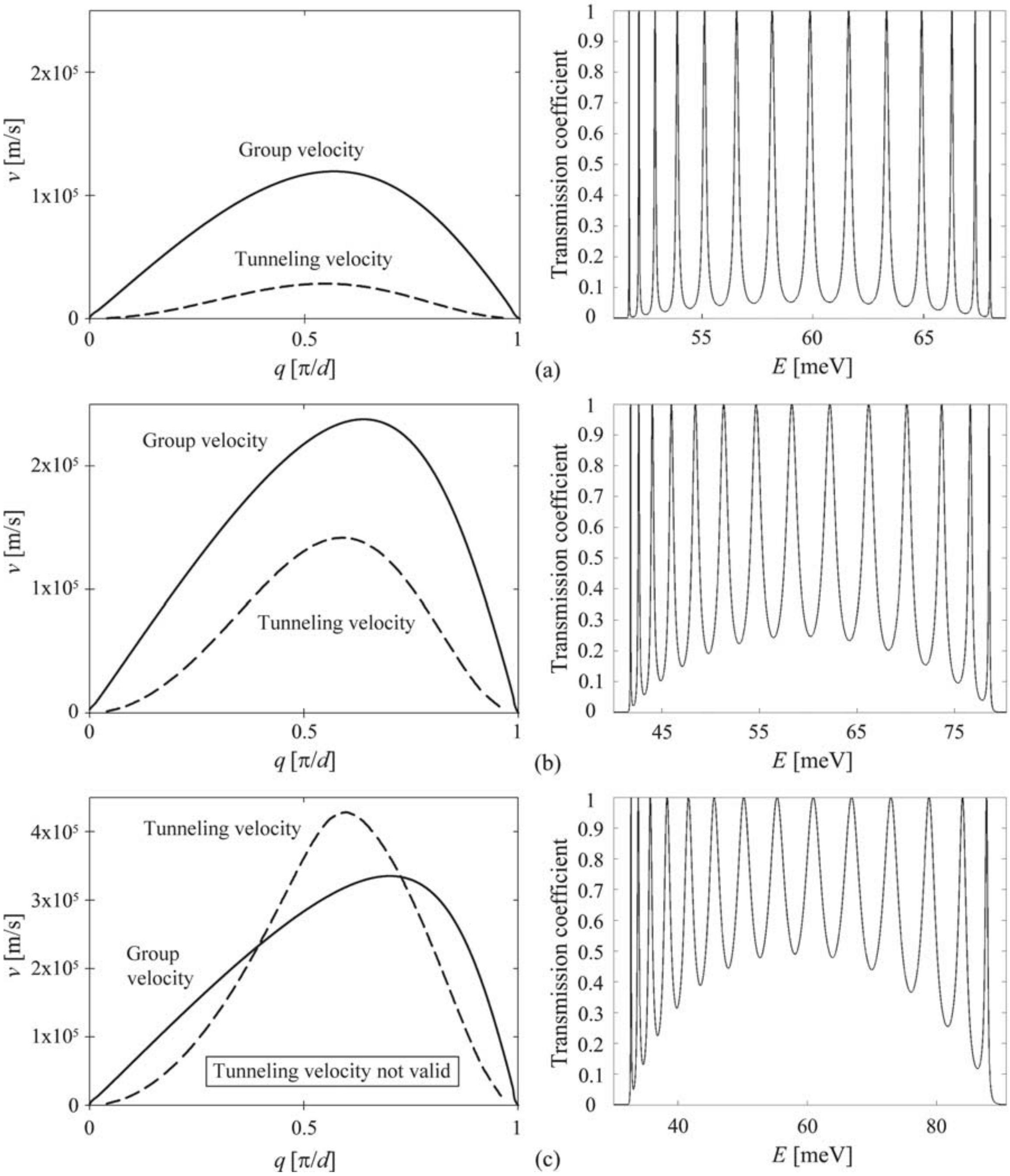

Fig. 4. Group velocity (solid line) and tunneling velocity, equation (6), (dashed line) vs. wave-vector of SLs with: (a) $b = 2.9$ nm and $w = 6.5$ nm; (b) $b = 1.7$ nm and $w = 6.5$ nm; and (c) $b = 1.1$ nm and $w = 6.5$ nm, respectively. On the right-hand side the corresponding transmission spectra for SLs with 15 periods are plotted. Since the shape of the transmission peaks deviates strongly from Lorentzian in Figure (c), the resulting tunneling velocity characteristic is not valid.

same. The decreasing of the outermost barrier widths increases the tunneling velocity, and vice versa. This demonstrates the strong influence of the boundary conditions on the tunneling velocity. Therefore, we conclude finally that the different boundary conditions of an infinite and a finite system lead to the difference between the group velocity and the tunneling velocity approach.

The whole treatment is in the context of coherent transport, and our results are only valid in this case, i.e. for structures which are shorter than the coherence length. In structures longer than the coherence length; scattering processes allow for redistribution of carriers, then the group velocity entering the Boltzmann equation is important for the calculation of the current density [2]. In the

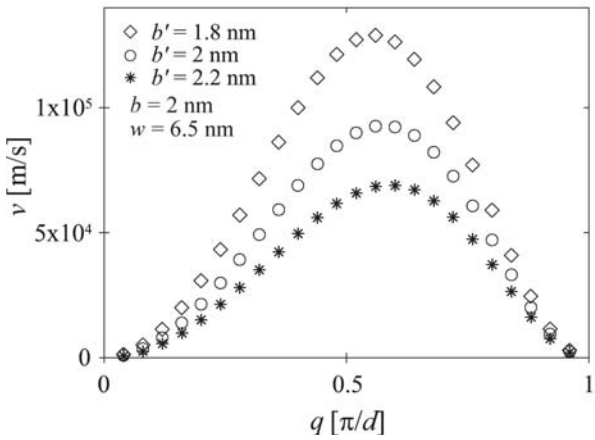

Fig. 5. Tunneling electron velocity in a SL with 25 periods where all barriers have width of $b = 2$ nm (circles) in comparison to SLs with $b = 2$ nm and outermost barrier widths of $b' = 2.2$ nm (asterisks) and $b' = 1.8$ nm (diamonds), respectively. The well widths are 6.5 nm throughout all three structures.

limit of structures much longer than the coherence length, without electric field applied, scattering processes lead to a homogeneous electron distribution in k-space. Then, at average contributions of electrons with positive and negative k-values (velocities) cancel out, leading to a vanishing current.

5 Conclusions

Our numerical analysis has shown a difference between the group velocity and the velocity defined through the tunneling time, equation (6), for coherent electron transport in superlattices. The calculation of the tunneling velocity in a finite weakly coupled SL can be performed by the following steps: i) calculation of the transmission spectrum of the SL (transfer matrix method), ii) determination of the HWHM of the resonance peaks in the spectrum, iii) calculation of the velocity using the tunneling time, i.e. equation (6). Compared to the group velocity this method has the advantage of taking into account the correct boundary conditions of the finite system. In the regime where the tunneling time can be derived from the HWHM of the transmission peaks the tunneling velocity is smaller than the group velocity. The group velocity was used to determine the electron mean free path from the scattering time (e.g. in undoped SLs [17,18]). Our results indicate that the tunneling velocity might be a more suitable choice, especially for weakly coupled SL where the differences can be appreciable.

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