Diffusive-Like Minibands in Finite Superlattices of Disordered Quantum Wells

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The existence of quantized levels, as a consequence of spatial confinement, does not necessarily imply in formation of superlattices minibands due to the coupling between these quantum wells. The present work discuss a framework to analyze the analoge to minibands in periodic superlattices made of disordered quantum wells. The inter quantum well coupling leads to diffusive-like minibands.

I Introduction

A model for a disordered quantum well (dQW) made of a short repulsive binary alloy (RBA) embedded by ordered barriers has recently been discussed [1]. Since in RBAs an effective delocalization window appears, the problem of delocalization in one dimensional chains [2, 3] could be addressed from the point of view of spatial confinement effects in such systems. These effects pose a new question concerning the coupling of dQWs in finite superlattices (SLs). Although well defined, the quantum well states show an inhomogeneous broadening due to the underlying disorder. Considering initially two coupled quantum wells, it is important to compare the energy scale of the inhomogeneous broadening to the tunneling splitting of the levels. If the broadening is of the order of (or larger than) this splitting, then the coupling of the quantum wells can not be resolved in the calculated energy spectra.

Here, we show that the coupling of quantum wells can be described by appropriate nearest level spacing statistics for an ensemble of SLs [4]. Furthermore, the level spacing statistics evolve to Poisson or Wigner surmise distributions in finite SLs, as a function of the localization lentgh, which depends on the SL miniband index. For sake of clearness, we will name as a miniband the level clustering around the average energy of a state in an isolated dQW. While one of the level clusters shows signatures of a true miniband, the others are characterized by either effectively extended or strongly localized states. The minibands of effectively extended states have level spacing properties of a diffusive-like regime.

II Model

Our Hamiltonian is a one-dimensional tight-binding chain of s-like orbitals, with nearest-neighbor interactions only, [1]

$$H = \sum_n \varepsilon_n |n><n| + V_{n,n+1}|n><n+1| + h.c. \quad (1)$$

The SL chain is constructed in a way that short RBAs, 40 atomic sites long, representing the quantum wells are separated by sets of $L_b = 2$, 3 or 5 sites for the barriers. In order to minimize surface effects, the chain ends are wide barriers. The tight-binding parameters used throughout this work are the same as in previous work [1]. The number of quantum wells in a finite SL varies in the range $2 \leq N_w \leq 50$.

In a RBA the bond between one of the atomic species is inhibited, introducing short range order: in a chain of A and B sites, only A-A and A-B nearest neighbors bonds are allowed. The well layer is therefore characterized by this correlation in disorder and the concentration of B-like sites, which is taken $\rho_B \approx 0.3$. Disorder is introduced by randomly assigning A and B sites, according to above constraints on concentration and bonding. Since we are simulating disordered systems, averages over 5000 configurations for the same parameters are undertaken.

III Results and discussion

a) Energy spectra and transmission probabilities

The analysis of the formation and the properties of minibands in disordered SLs is a non trivial task, because the standard framework (Bloch theorem) for studying minibands is lost. However, this may be done with usual tools, namely the energy spectra and transmission probabilities.

In Fig.1 we show the energy spectra as a function of the configuration, for single, double quantum wells and 5 dQWs, with $L_b = 2$. Only the spectra in the range around the energy of maximum localization length of an infinite RBA, $\lambda_{max} \approx -0.7eV$ [1] is shown. According to the parameters and the well width, the bona fide quantum well states correspond to the index $n = 11$, $n = 12$ (indicated by an arrow) and $n = 13$. For a wide tight-binding parameters range and barriers widths down to $L_b = 2$ sites, we are dealing with the interesting limit where the average level repulsion turns up to be of the order of the inhomogeneus broadening of QW levels.

These level clusters, minibands, are related to states that are still well defined quantum wells states and should repeal each other due to quantum well coupling. If these level clusters have features of a true miniband like in ordered systems, will depend on whether it is possible to determine a level repulsion due to quantum well coupling. However, such level splitting is not resolved in the average energy spectra, even in the case of a double-well with very thin barriers.

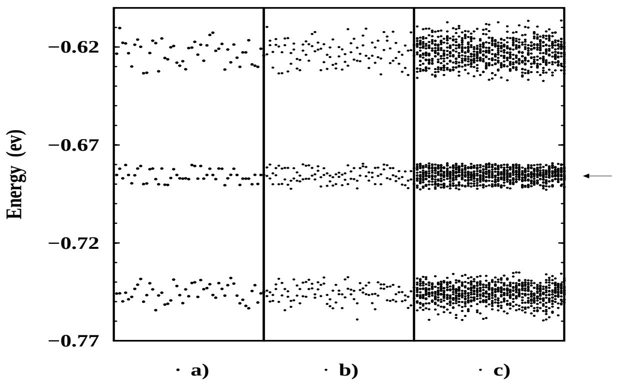

Figure 1. Energy spectra for 50 different configurations: (a) for a one; (b) two; and, (c) five disorder quantum well.

Resonances in the transmission probability, through quantum well systems are spectroscopic probes of their quasi-bond states. The transmission probability through finite disordered SLs can be obtained within the given model, using the transfer matrix approach [1]. Fig. 2 shows the average transmission probability versus energy for some finite SLs: (a) for 3, (b) 5 and (c) 15 coupled quantum wells. The resonance marked by an arrow corresponds to the $n = 12$ miniband. We clearly observe resonant transmission bands in these disordered systems.

Having both Figs. 1 and 2 in mind, it becomes clear that neither internal structure of the minibands can be resolved nor the minibands become wider with increasing the number of QWs in the SL, as expected for ordered systems. This is characteristic of a situation where the inhomogeneus broadening is larger than the level repulsion due to the QWs coupling. The reduction in the fluctuations, on the transmission probabilities, with increasing the SL length may be attributed to a better ensemble average for large systems. The existence or not of coupling between the QWs can only be verified by level spacing distribution.

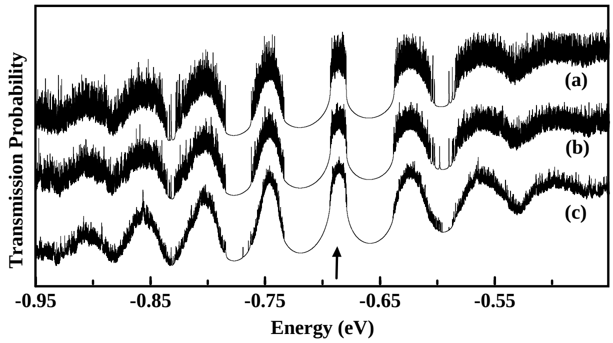

Figure 2. Average transmission probability through finite disordered SLs. a), 3; b), 5; and c) 15 quantum wells.

b) Level spacing distributions

The level spacing statistics within a given miniband is a well defined problem, since the eigenvalues clusters deliver sets of equal number of levels with comparable localization lengths and these sets are well separated in energy from each other. In other words, a finite SL overcomes the problem of arbitrarily defining energy intervals where to evaluate the level spacing distributions, in opposition to long one-dimensional chains with correlated disorder [5] showing an almost continuous spectrum of states with localization lengths that are strongly energy dependent [6].

Nearest neighbor level spacing distributions for 6 coupled dQWs are shown in Fig. 3. We consider two different barrier widths, $L_b = 2$, left panel, and $L_b = 3$ sites, right panel for the $n = 13$, (a), $n = 12$, (b) and $n = 11$, (c), minibands. Histograms obtained numerically are compared to analytical Poisson and Wigner distributions. The later are evaluated with the corresponding numerical average level spacing, D.

The nearest neighbor level spacing distribution for thin barriers approaches a Wigner distribution, as can be seen in the left panel of Fig. 3, which is expected for correlated levels. By increasing the barrier thickness, the minimal level splitting diminishes exponentially becoming negligible when it is compared to the average level spacing. In this limit, actually seen for $L_b = 3$, (right panel of Fig. 3) the nearest neighbor level spacing distribution approaches to Poisson distribution, which is expected for uncorrelated states, *i.e.* localized in only one of the wells.

On the other hand, in the right part of Fig. 3(b), for the $n = 12$ states, there are structures in the level spacing distribution. Here no definitive answer, concerning the correlation of levels, can be delivered from comparisons with either Wigner surmise or Poisson distributions. In this miniband the level broadening is the smallest one, since its energy is almost perfectly tuned to the energy of maximum localization length of an infinite RBA, $\lambda_{max} \approx -0.7eV$. Therefore, some memory of the corresponding ordered system, with enhanced level repulsion, should be the origin of these clear deviations of a Wigner surmise.

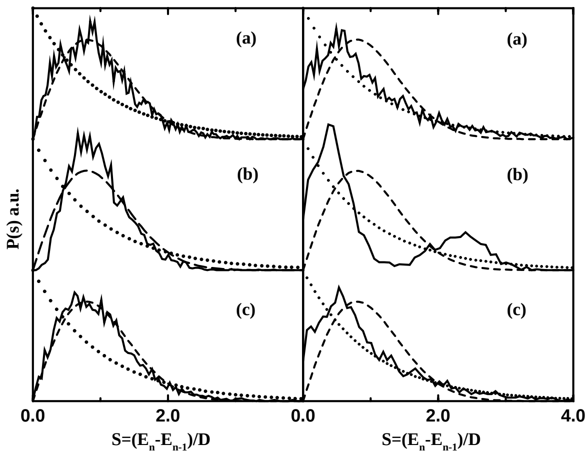

Figure 3. Nearest level spacing distribution for central levels at n=13, (a), n=12, (b), and n=11, (c), minibands of finite SLs with 6 dQWs. Poisson distributions (dotted lines) and Wigner (dashed lines) surmises, for the respective average nearest level spacings, are also shown. Left (Right) panel: $L_b = 2$ ($L_b = 3$) .

A transition to localization with increasing the SL length can be seen in the level spacing distributions for the $n = 12$ miniband. In Fig. 4, results for SLs with 10 (a), 30 (b), and 50 (c) dQWs are displayed: left (rigth) panel for levels at the center (edge) of the miniband. In the both cases, the level spacing distribution shows a transition from Wigner to Poisson distribution. For small spacings, this transition is slower than for large ones. Is is expected that for even longer SLs the level spacing distribution would approach a Poisson distribution, irrespective of the level spacing.

The present results show minibands whose level spacing distributions are close to Wigner surmise. This implies that the related localization length, λ, is larger than system length, L. On the other hand, in one-dimensional systems, the elastic mean free path l is of the order of the lattice parameter a. Therefore, $l < L < \lambda$, which is characteristic of a diffusive regime. Furthermore, not all the states in a miniband are effectivelly extended. For these reasons we call it as diffusive-like minibands. A whole miniband is neither in the localized regime (pure Poisson distribution) nor in the ballistic regime (true minibands).

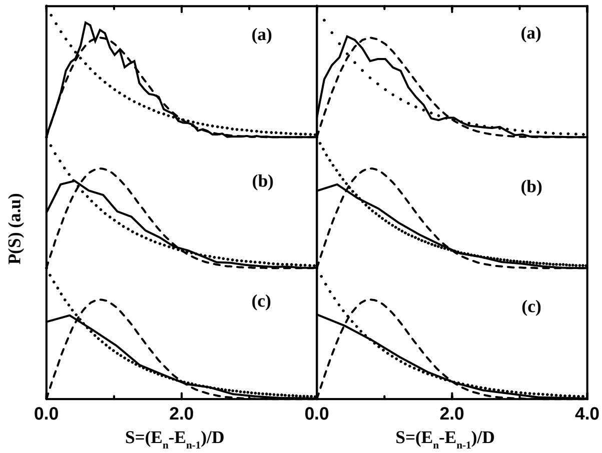

Figure 4. Nearest level spacing distribution for central (left panel) and edges (right panel) levels of n=12 minibands for finite SLs 10, (a), 30, (b), and 50, (c), dQWs. Poisson distributions(dotted lines) and Wigner (dashed lines) surmises.

IV Conclusions

The present model constitutes a potentially interesting tool for analyzing regular superlattices made of disordered materials, where a mobility edge may play an important role, like in amorphous semiconductor superlattices [7]. The mobility edge is emulated by the delocalization window in the energy spectra of RBA as has been discusssed.

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