Level spacing statistics of disordered finite superlattices spectra
and motional narrowing as a random matrix theory effect

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Abstract

In the present work the problem of coupled disordered quantum wells is addressed in a random matrix theory framework. The quantum wells are short repulsive binary alloys embedded by ordered barriers and show well defined quantized levels as a consequence of spatial confinement. Finite disordered superlattices may show both diffusive-like and localized minibands. Three different level repulsion suppression mechanisms are discussed by analysing the evolution of nearest-level-spacing distribution function within each superlattice miniband. The present numerical results show a motional narrowing effect, which is in fact a consequence of the random matrix theory.

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I. INTRODUCTION

In a recent work we discuss a model disordered quantum well made of a short repulsive binary alloy embedded by ordered barriers [1]. Since repulsive binary alloys show a correlation in the disorder, an effective delocalization window could be established in the energy range below the barrier top. Therefore, the intensively studied problem of delocalization in one-dimensional chains with correlated disorder [2–11] could be addressed from the point of view of quantization effects due to spatial confinement in such chains. A further motivation concerns the verifiability of quantum confinement effects in amorphous semiconductor heterostructures, a largely unanswered question [12,13]. In this context repulsive binary alloy quantum wells lead to a description of these systems including inherently a key feature of many disordered bulk materials: the presence of well defined energy ranges showing either localized or effectively delocalized states [14].

The existence of well defined spatial confinement quantization in these model disordered quantum wells poses a new question concerning the coupling of quantum wells in finite superlattices. Although well defined, the quantum well states show an inhomogeneous broadening and therefore it is not clear how the level repulsion due to quantum wells coupling behave as a function of the localization length. Once the coupling of two disordered quantum wells by means of tunneling through a barrier could be described, the evolution of level repulsion in finite superlattices could show still qualitative different aspects.

In the present paper we show that the coupling of two quantum wells can be well described by the usual tunneling mechanism in a picture delivered by appropriate level spacing statistics for an ensemble of double quantum wells. Furthermore, the level spacing statistics evolve to Poisson or Wigner surmise distributions [15] in finite superlattices, depending on the miniband index. For sake of clearness, in the present work we will name as a miniband the level clustering around the average energy of the levels of isolated quantum wells. Hence, level spacing statistics will be applied for levels within a given miniband. Therefore, for a given set of parameters, while one level cluster may show signatures of true minibands [16],
others present from an effectively extended behaviour down to strong localization in the
same superlattice. The minibands of effectively extended states have level spacing prop-
erties of a diffusive-like regime. We also identify in the present system a motional narrowing
effect in difusive-like minibands, which is actually a consequence of random matrix theory
(RMT) [17].

In what follows we first describe briefly the model Hamiltonian for the disordered quan-
tum wells and finite superlattices, as well as the level spacing statistics approach. After-
wards results for finite disorder superlattices spectra will be shown and discussed based on
the nearest neighbour level spacing statistics properties. Finally, the numerical results for
the motional narrowing effect will be presented and analysed as a consequence of RMT.

II. DISORDERED FINITE SUPERLATTICE MODEL HAMILTONIAN

The present model Hamiltonian consists of a one-dimensional chain of $s$-like orbitals,
treated in the tight-binding approximation, with nearest-neighbor interactions only,
$$H = \sum_n (\varepsilon_n |n> < n| + V_{n,n+1}|n> < n+1| + V_{n+1,n}|n+1> < n|),$$

(1)

A finite chain segment will emulate a single well, or a finite superlattice, sandwiched by
infinite barriers (isolated structure). The actual chain is constructed in a way that short
disordered segments representing the quantum wells are separated by sets of few sites for
the barriers. The ends of the total chain segment will emulate wider barriers, of same high
as the internal ones, in order to minimize surface effects at the quantum wells at the ends
of the finite superlattices.

The well material is the above mentioned repulsive binary alloy [3,4], where 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 introduction of
this short range order leads to delocalization of states in the disordered chain [11,14]. The
well layer is then characterized by the correlation in disorder and the concentration of $B$-like
sites, which is related to the probability $P_B$ of a $B$-like site to be the next one in generating a particular chain configuration. All results shown here are for $P_B = 0.5$, corresponding to an effective concentration of $B$-like sites of $\rho_B \approx 0.3$. Disorder is straightforwardly introduced by randomly assigning $A$ and $B$ sites, according to the constraints on concentration and bonding mentioned above. Since we are simulating disordered systems, averages over hundreds of configurations for the same parameters are undertaken.

The atomic site energies used throughout this work are $\epsilon_A = 0.3$ eV, $\epsilon_B = -0.3$ eV and the hopping parameter are $V_{AA} = -0.8$ eV between $A$-like sites and $V_{AB} = -0.5$ eV between $A$-like and $B$-like sites for the well layer [14]. For the barriers these parameters are $\epsilon_{br} = 0.8$ eV and $V_{br} = -0.4$ eV. The results shown here are all considering wells of $L_w = 40$ sites and barriers widths of $2 \leq L_b \leq 15$ sites. The external barriers are characterized by the same barrier parameters given above and are $L_{ext} = 11$ sites wide. At interfaces we consider geometric averages of the hopping parameters. The number of quantum wells in a finite superlattice is varied in the range $2 \leq N_w \leq 19$, throughout the present work.

**III. LEVEL SPACING STATISTICS**

A bona fide quantum well state in a single disordered quantum well still shows an inhomogeneous broadening due to the underlying disorder, related to a finite localization length, even if this length is many times longer than the well width, a condition necessary for the spacial quantization itself. On the other hand, considering two coupled quantum wells, it is important to compare the energy scale of this inhomogeneous broadening to the tunneling splitting of the levels. A level splitting must be determined as an average over several double well like chains with different disorder configurations. However, if the broadening is of the order of (or larger than) this splitting, then the coupling of the quantum wells can not be resolved numerically in an average of the energy spectra. We will see that this is actually the most common situation we found by numerical inspection of the problem. Therefore we must consider a nearest neighbour level spacing statistics of the spectra.
Having in mind the double-well system, we refer to the coupling between the quantum wells as a two level problem [18] and the splitting $S$ is given by

$$S^2 = (H_{11} - H_{22})^2 + (2 \cdot H_{12})^2 \tag{2}$$

where $H_{11}$ and $H_{22}$ are the energies of equivalent quantized levels, one in each well, while $H_{12}$ is the coupling between both wells. If $H_{11} - H_{22}$ and $2H_{12}$ are independent Gaussian random variables, the distribution of the level spacing (tunneling splitting) is given by a Wigner surmise:

$$P(S) = \frac{\pi}{2D^2} S \exp\left\{-\frac{\pi}{4} \frac{S^2}{D^2}\right\} \tag{3}$$

where $D$ is the average spacing. If $H_{12} = 0$, i.e., there is no coupling between the states of the two quantum wells, the distribution of the level spacing reduces to the Poisson distribution:

$$P(S) = \frac{1}{D} \exp\left\{-\frac{S}{D}\right\} \tag{4}$$

The average level spacing, $D$, is related to the variance, $\sigma^2$, of the Gaussian random variables by $D = \sigma \sqrt{\frac{2}{\pi}}$ [18]. These are two interesting limits given by RMT which establish a useful investigation tool for the coupling between two (or more) disordered quantum wells, relative to the localization length in these systems [19]. It should be noticed that, while $H_{11} - H_{22}$ is a random variable, since there is a inhomogeneous broadening of the levels; $2H_{12}$ is not entirely random for a few quantum wells system. In what follows we will show that numerical results confirm this prediction, but the coupling between wells will be independently randomized in multiple coupled quantum wells and the Wigner surmise will also become an important limit of the general problem.

The level spacing statistics for levels within a given miniband is a well defined problem, since the clustering of eigenvalues in minibands delivers sets of equal number of levels of comparable localization lengths and these sets are well separated in energy from each other. In other words, a finite superlattice overcomes the problem of arbitrarily defining energy...
intervals where to evaluate the level spacing distributions, like in long one-dimensional chains with correlated disorder \cite{20} showing an almost continuous spectra of states with localization lengths that are strongly energy dependent \cite{21}.

IV. ENERGY SPECTRA AND LEVEL SPACING DISTRIBUTIONS

Previous results on single disordered quantum wells \cite{1} show that quantum confinement effects are already resolved if some average level spacings are greater than the level broadening. However, the formation of superlattice minibands with the successive coupling of disordered quantum wells is related to a different energy scale. In order to build up a miniband of Bloch states, the inhomogeneous level broadening has to be much less than the level repulsion due to the tunneling coupling. For a given tight-binding parameters set this quantum well level splitting can be tuned by changing the barrier width. After several numerical tests we chose the parameters listed in section II. For the most favorable situation found for barrier widths down to $L_b = 2$ sites, the average level repulsion turned out to be of the order of the inhomogeneous broadening of the levels, with the exception of a peculiar quantum well level, as will be discussed below.

In Fig.1 we show the energy spectra as a function of disorder configuration, for a single quantum well, a double quantum well and a finite superlattice of five quantum wells, for $L_b = 2$. The spectra are shown in the range around the energy of maximum localization length of an infinite repulsive binary alloy with the given parameters, $\lambda_{max} \approx -0.7eV$ \cite{14}. We can see an internal structure for the level $n = 12$, that partially survives in the double quantum well and in the finite superlattice, with clear signatures of level splitting due to quantum well coupling. For a finite superlattice this intra-miniband structure is better observed in the level-spacing distribution, as will be seen below. This quantum well level is closely tuned to the $\lambda_{max}$ energy for a $L_w = 40$ sites well. Hence, the level broadening is the lowest one, leading to the resolution of the internal structure of the average level spectrum. This structure is related to the fact that the well is a repulsive binary alloy and the effective
well width varies according to the interface sites. Three different configurations at the interface are possible: (a) A-like site at both interfaces, (b) one A-like site at one interface and a B-like at the other; (c) and B-like sites at both interfaces. The localization increases from (a) to (c), proportional to the detuning of the $\lambda_{\text{max}}$ condition and the consequent increase in the inhomogeneous broadening. The level repulsion for these $n = 12$ states is partially resolved on average for a double-well. Nevertheless, increasing further the number of wells, the average energy separation of nearest neighbour levels within a miniband decreases and the coupling among quantum wells is not resolved anymore for a finite superlattice, as can already be seen for finite superlattice of five quantum wells. The miniband immediately below, related to the level $n = 11$, has an inhomogeneous broadening already wider than the internal average structure due to the interface configuration. On the other hand, these states are still bona fide quantum wells states and should repeal each other by quantum well coupling, but such level splitting is not resolved in the average spectrum even in the case of a double-well with very thin barriers, Fig.1.

The level splitting for these states may actually be quantified in histograms of individual levels of the $n = 11$ doublet, Fig. 2. In Fig. 2(a) the histograms generated by the lower and the higher state taken separately in 1000 disorder configurations are depicted. Each level shows a nearly Gaussian inhomogeneous broadening with a half width of the order of the average level splitting given by the energy separation of curve peaks, $\delta$. The average density of states in this energy range, Fig. 2(b), on the other hand, is structureless, as mentioned above. Since disordered quantum wells states show a coupling, but with a level splitting of the order or less than the individual level broadening, the density of states is not a useful quantity to be analysed and one should look at the nearest neighbour level spacing statistics.

Nearest neighbour level spacing probabilities for double disordered quantum wells are shown in Fig.3. We consider the $n = 12$, Fig. 3(a); and $n = 11$, Fig. 3(b), doublets. The numerical histograms, obtained taking into account 1000 disorder configurations, are compared to analytical Poisson and Wigner distributions for the numerically obtained average
level spacing, $D$. Here we also consider different barrier thicknesses, $L_b = 2$ and $L_b = 5$
sites wide, as a mechanism that modify the level repulsion. First, for thin barriers (strong
coupling), top of Fig. 3(a) and 3(b), we see that the level spacing probabilities present a
threshold, $\Delta$, for both doublets. This threshold, i.e., the minimum value for level spacing, is
a direct measure for the tunneling coupling between resonant states. This can be confirmed
by inspecting that indeed $\ln \Delta \propto -L_b$. The spacing probability for the $n = 12$ doublet show
a rich structure above the threshold, which is due to the resolved interface related structure,
already seen in the energy spectra as a function of disorder configuration, Fig. 2. For the
$n = 11$ states the spacing probability distribution is a smoother structureless curve, which
is an evidence for an level broadening wider than the level repulsion.

This picture changes completely for thicker barriers. By increasing the barrier thickness,
the minimum level splitting diminishes exponentially, becoming negligible compared to the
average level spacing. In this limit, already seen for $L_b = 5$, the nearest neighbour level
spacing approaches a Poisson distribution, as can be seen in the bottom panel of Fig. 3(b),
which is expected for uncorrelated levels, localized in either one of the wells. In the bottom
part of Fig. 3(a), for the $n = 12$ (more delocalized) states, there are still structures in the
level spacing distribution and no definitive answer concerning the correlation of levels can be
delivered from comparisons with either Wigner surmise or Poisson distributions. Interesting
to notice is the fact that no Wigner surmise like distribution is obtained in the thin barrier
limit. Although the almost degenerate levels show a Gaussian random distribution, the
coupling between them is not random. The finite threshold shown in the top of Fig. 3(b)
actually suggests that the coupling is nearly constant in a first order approximation.

Inter-well coupling, however, may be randomized if we increase the system by adding
successive quantum wells, generating a finite superlattice. With such a procedure, the level
repulsion diminishes linearly and not exponentially and a Wigner like distribution could
be expected. This trend can be already observed for a finite superlattice of five quantum
wells, keeping the barrier width $L_b = 2$, Fig. 4. In this figure the level spacing for other
minibands of more localized states are also depicted: (a) for the \( n = 12 \) miniband; while (b), (c), and (d) are for the \( n = 11 \), \( n = 10 \), and \( n = 9 \) minibands, respectively. Now we see that the miniband related to \( n = 12 \), although showing some structure, presents a clear Wigner surmise envelope. For low spacing, however, a threshold is still seen. This threshold is already absent for the other minibands in this five quantum wells finite superlattice. For the \( n = 11 \) states related miniband, the numerical simulation of level spacings shows a perfect agreement with the Wigner surmise distribution. This agreement is still reasonable for the \( n = 10 \) miniband, Fig. 4(c), while for lower miniband indexes, like in Fig. 4(d), a crossover from Wigner surmise to Poisson distribution is clearly identified.

The fact that in a finite superlattice of disordered quantum wells, nearest neighbour levels associated to the same minibands obey a Wigner surmise indicates that these levels are still correlated and extended along the entire system, Fig. 4(b). Besides, we may determine a lower bond for the localization length of these states: as far as the level spacing in a given miniband follows the Wigner surmise, the localization length exceeds the system length, \( \lambda > L^{[15]} \). Based on this evidence, further increasing of the system length, by adding more quantum wells, would lead to a transition to localization, i.e., \( \lambda < L \).

The transition to localization with increasing the number of quantum wells can be seen for the level spacing distribution of a fifteen wells long superlattice, Fig. 5: (a) for the \( n = 12 \) miniband and (b) for the \( n = 11 \) miniband. In this figure we also pay attention to the difference in level spacing distribution for level at the center of a miniband, top of Fig. 5, and at the edges, bottom of Fig. 5. For \( n = 12 \) states at the center of the miniband, top of Fig. 5(a), the level spacing distribution still follows a Wigner surmise. A clear transition to a Poisson distribution is seen for the level spacing at the bottom edge of the miniband (bottom of Fig. 5(a)). The transition towards localization is already seen for levels at the center of the \( n = 11 \) related miniband. Due to the inhomogeneous broadening of the quantized levels there is no miniband formation in the usual sense of ordered systems which could be characterized by a near clean or at least a ballistic regime \([22,23]\). Nevertheless, minibands in a less strict
sense are defined by a set of states which repeal each other and are delocalized through the whole system.

These results suggest that finite superlattices of quantum wells with correlated disorder present very interesting properties related to the competition between the level repulsion and the level broadening. Such a competition can be defined for the fact the inhomogeneous broadening is mainly related to the properties of the repulsive binary alloy from which the quantum wells are made of, while the level repulsion is introduced by the coupling of the quantum wells, which can be partially tuned through more or less transparent barriers. From this point of view, the transition from diffusive-like regime to a localized one may be obtained by means of three different mechanisms.

The first mechanism is the suppression of level repulsion by increasing barrier widths, illustrated for the double-well case in Fig.3. By increasing the barrier width, the coupling between the wells is reduced and the states tend to localize in only one of the wells. Here we see that the tunneling range depends on the inhomogeneous broadening of the almost resonant states. For barriers wider than the tunneling range, the states become uncorrelated. In other words, varying the barrier width, introduces a spatial dependence of the density correlation function in analogy to the energy-level correlation function analysis for the Anderson disordered tight-binding model by Sivan and Imry [24].

A second mechanism of coupling suppression is simply related to the localization properties of the bulk chain that constitutes the material disordered quantum wells. Hence, for a given superlattice, there are minibands with different degrees of localization, from clusters of states with true minibands characteristics to completely localized ones, including at least one miniband with a diffusive character. This effect can be followed for the different minibands of a five well superlattice in Fig.4.

Probably the most interesting repulsion suppression mechanism is related to increasing superlattice length. Related to this mechanism is the expected behaviour that a diffusive-like miniband in a finite superlattice becomes localized, if the number of quantum wells makes
the superlattice exceed the localization length for this given miniband. The level spacing statistics evolve from a Wigner surmise towards a Poisson distribution because some levels start to become uncorrelated. This behaviour can be identified by comparing Fig.4 with Fig.5.

On average, the level repulsion within a miniband decreases with the increase of the number of quantum wells in a superlattice. This follows the textbook picture within a tight-binding framework, of the formation of continuous bands for infinite crystals by the successive addition of atoms to the system.

V. MOTIONAL NARROWING

Although the suppression of level repulsion with increasing the number of quantum wells can be identified in the level spacing statistics, a more precise signature of this mechanism is related to a motional narrowing effect. The term "motional narrowing" has been used to designate the reduction of spectral line widths in disordered systems by some averaging process. Such effect occurs in many areas of physics and, in particular, has recently been predicted and observed in semiconductor microcavities. In the present work, the motional narrowing shows up as a diminution of the inhomogeneous broadening of the states with increasing the system length. In Fig. 6 the average histograms of individual levels of the \( n = 11 \) miniband for superlattices of different length are shown; \( N_w = 5 \), Fig. 6(a); and \( N_w = 9 \), Fig. 6(b). It is noticeable the shrinking of the average half width of the states with increasing the number of quantum wells. For a better comparison, we pay special attention to the central miniband state in either case. Actually the narrowing of the broadening is more intense for this state. This narrowing may be qualitatively understood by the fact that the level repulsion inhibits the inhomogeneous broadening of an individual level taken as an average over many disorder configurations, since the levels in a finite superlattice are correlated. In other words, coupling of states shrinks the range for broadening and the central state in a miniband feels the strongest reduction of this broadening range. In a more
precise way, this motional narrowing effect is predicted by the RMT, having in mind the expression for the Wigner surmise. The average level repulsion, \( D \), in eq. (3) is directly related to the half width of the random gaussian distribution of \( H_{ij} \) in eq. (2), \( D = \sigma \sqrt{\frac{2}{\pi}} \). A finite disordered superlattice is characterized, in analogy to the ordered counterpart, by the reduction of the average level repulsion with increasing system size. This reduction leads to a diminution of the broadening of the random distribution of the Hamiltonian matrix elements. Hence, the motional narrowing is an effect directly related to and explained by the RMT.

VI. CONCLUSIONS

The present model for a finite superlattice overcomes the usual difficulties of RMT applied to one dimensional systems. Furthermore, the transition from Wigner surmise to Poisson, by increasing the system length, suggests that some minibands - although defined in a one-dimensional system - show properties of diffusive regimes. Important here is the presence of correlations, as well as the limit of states completely isolated in a single quantum well and the natural localization length selection by the miniband index. However, there is also a fine tuning of the localization length in each miniband, as can be seen already from the differences in level spacing distribution for different level pairs within a miniband, as depicted in Fig. 5. Further, a less pronounced motional narrowing for states at the edges of a miniband, compared to central ones, is also an indication of this localization length tuning. A definitive result for the modulation of the localization length within a miniband is given by the participation ratio \[ P = \sum_{\vec{r}} |\Psi(\vec{r})|^4, \] (5)

where \( \| \Psi \| = 1 \). In the tight-binding model with \( N \) atomic sites eq. (5) becomes:

\[ P = \sum_{i=1}^{N} |a_{\alpha i}|^4 = A_{\alpha} \] (6)
where $a^\alpha_i$ is the $i$th site component of $\alpha$ eigenstate.

The participation ratio, $P$, is inversely proportional to the localization length \[21\]. Besides, the participation ratio delivers an overview of the main results shown in the present paper. In Fig. 7, the average participation ratio for $N_w = 19$ superlattices are shown. Open circles are for thin barriers, $L_b = 2$ and full squares for thick barriers, $L_b = 5$. For both cases, several minibands separated by minigaps are identified. However, only for the thin barrier case, the minibands show a clear behaviour of the centre less localized than the edges. This recalls the mechanism of suppressing level repulsion by increasing barrier width. We also observe the reduction of localization length together with increasing broadening for minibands progressively away in energy from $n = 12$ miniband, recalling the behaviour of the localization length of a repulsive binary alloy bulk chain. It should be noticed that for energies below -0.85 eV and above -0.5 eV in Fig.7, no minibands are resolved in the energy spectra. Nevertheless a clear modulation of the localization length is still present. This suggests that minibands in disordered superlattices could be still defined by a modulation of the localization length in a continuous spectrum.

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FIGURES

FIG. 1. Part of the energy spectra for 100 different disorder configurations: (a), for a single quantum well; (b), for a double quantum well; and, (c), for a finite superlattices of five quantum well. For other structure parameters, see text.

FIG. 2. (a) Histograms of energy distributions for the lower and upper level of the n=12 doublet of a double disorder quantum well. (b) Average density of states for the same n=12 doublet in (a). Quantum well parameters are the same as in Fig. 1(b).

FIG. 3. Nearest level spacing distribution for the n=12, (a), and n=11, (b) doublet of a double disorder quantum well for different central barrier thickness: Top for thin, $L_b = 2$ sites, barriers; and bottom for thick, $L_b = 5$ sites, barriers. Poisson distribution (dashed lines) and Wigner (dotted lines) surmise are also shown for comparison.

FIG. 4. Nearest level spacing distribution for n=12, (a), n=11, (b), n=10, (c), and n=9, (d), minibands of a finite superlattices of five quantum wells. Poisson distributions(dashed lines) and Wigner (dotted lines) surmises, for the respective average nearest level spacings, are also shown for comparision.

FIG. 5. Nearest-neighbour level spacing distributions for the n=12, (a), and n=11, (b), minibands of a fifteen quantum wells finite superlattice. Top: distribution for central levels in the miniband. Bottom: distribution for levels at the bottom of the miniband. Poisson distributions (dashed lines) and Wigner (dotted lines) surmises are also shown.

FIG. 6. Energy histogram for individual levels of the n=11 miniband for finite superlattices: (a) five quantum wells; and (b), nine quantum wells. Thick lines corresponds to the center level in these minibands.

FIG. 7. Participation Ration as a function of energy for a finite superlattice of nineteen disordered quantum wells. Different barrier thicknesses are considered: $L_b = 2$ sites (open circles), and $L_b = 5$ sites ( full squares).
\[ w = \frac{(E_n - E_{n-1})}{D} \]

The figure shows the probability distribution \( P(w) \) for different values of \( L_b \). The graphs are labeled as (a) and (b) with \( L_b = 2 \) and \( L_b = 5 \) respectively. The x-axis represents \( w = \frac{(E_n - E_{n-1})}{D} \).
\( w = \frac{E_n - E_{n-1}}{D} \)

(a) (b) (c) (d)
\[ w = \frac{E_n - E_{n-1}}{D} \]

(a) (b)
