Density of states for a weakly coupled disordered array

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A technique for the calculation of the density of states for a one-dimensional array of rectangular quantum wells in the weak-coupling limit is described, at various degrees of disorder. It is found that in the limit that the degree of disorder grows large, the smooth component of the density of states of this configuration is well approximated by the polynomial function

$$D(\varepsilon)=7.4-1.8\varepsilon+0.50\varepsilon^2-0.098\varepsilon^3,$$

where ε represents the absolute value of energy measured in units of $10^{-4}\hbar^2/2ma^2$, m is particle mass, and a is well width. The function $D(\varepsilon)$ exhibits a localization of energies at the maximum bound-state energy $\varepsilon=0$. A calculation is included which addresses the distribution of nearest-neighbor spacings of energies for the present configuration. The distribution obtained illustrates strong attraction between eigenvalues and is found to be well approximated by an exponential (Poissonian) fit.

I. INTRODUCTION

One-dimensional modeling has found wide application in superlattice study[1–5] and the modeling of the Mott and Anderson metal-insulator transitions.[6–11] In the latter area, one speaks of glass (or liquid) vs alloy one-dimensional models. In the glass model, quantum wells of the array are identical with wells randomly displaced from one another. In the alloy model, interwell displacements are equal to potential-well depths randomly distributed. A study of the density of states likewise divides into two categories: vibrational[12–14] and electronic.[15] Attention has also been given to Fibonacci,[16] as well as Thue-Morse[17,18] superlattices. In works closely allied with the present analysis, the density of states for a one-dimensional disordered array of δ-function potentials were studied[19–22] and employed in the modeling of impurities in a semiconductor. The resulting density of states is relevant to interactions, each of which have only one bound state and thus cannot readily be compared to the present findings.

The present work addresses the smooth component of the density of electronic states for an alloy configuration in the weak-coupling approximation, in which electrons are localized at quantum-well sites with negligible wave-function overlap.[23] A technique of analysis is introduced, based in large part on a graphical display of energies. In the ensuing numerical work, a polynomial expression for the density of states is obtained for varying degrees of disorder of the potential array. In the limit that the degree of disorder grows large, this polynomial expression is found to more accurately fit the density of states.

The measure of disorder in the present study is given by the number N of uniformly distributed distinct potential-well depths in a given array. Four values of N were considered, ranging from $N=100$ to 4500. For any choice of N, the resulting density expression is appropriate either to the ensemble average density for a disordered array of N quantum wells with N varying potential depths, or an infinite chain of quantum wells with N varying potential depths randomly distributed over the potential array.

A calculation is included addressing the distribution of nearest-neighbor spacings of energies for the present configuration. The distribution obtained illustrates strong attraction between eigenvalues and is found to be well approximated by an exponential (Poissonian) fit. This observation is an example of the extension of the application of the Berry-Tabor theorem[24] to one-dimensional motion.

As noted above, the present analysis is valid in the weak-coupling approximation, in which electrons are localized at individual quantum-well sites with virtually no coupling between wells. It should be noted that with finite coupling between quantum wells, as described in the linear combination of atomic orbitals (LCAO) approximation, energy levels split about unperturbed values. As the coupling approaches zero, the splitting of levels also goes to zero. Thus, for infinitesimal coupling, energy levels closely resemble those of isolated wells. With this observation, one may infer that the present analysis offers a reasonable approximation for the density of states in the given weak-coupling limit.

II. ANALYSIS

A. Review

In a previous work by the authors,[25] an analytic expression for the energies of $N\geq 1$ coupled, common quantum wells was obtained. This dispersion relation appears as

$$g_{\pm}(f,N,\xi,\eta)=0\ , \tag{1a}$$

$$\xi^2+\eta^2=\rho^2\equiv\frac{2ma^2V}{\hbar^2}\ , \tag{1b}$$

$$|E| = \frac{\hbar^2 \eta^2}{2ma^2} \ . \tag{1c}$$

In these relations (a, V) represent the width and depth of a well, respectively, E is energy, $f \equiv b/a$, where b is displacement between wells, and $\xi \equiv ka, \eta = \kappa a$, where k and κ are propagation and decay constants, respectively. The $(\pm)$ subscript in (1a) refers to even and odd eigenstates, respectively, whereas g is a composite function of transcendental forms.

It was observed in Ref. 25 that, for $f > 0.5$, quantum wells are very weakly coupled. In this limit, (1a) reduces to

$$g_{\pm}(\xi, \eta) = 0 \ , \tag{2}$$

which are the well-known dispersion relations[26]

$$(+)\eta = \xi \tan(\xi/2) \ , \tag{3a}$$

$$(-)\eta = -\xi \cot(\xi/2) \ . \tag{3b}$$

Note in particular that the relations (3) are universal to all quantum wells of width a, independent of the depth of a given well. Note also that these relations are appropriate to a single isolated well or a set of $N > 1$ uncoupled wells.

Thus, for example, consider the case of five wells at $f > 0.5$, and at varying depth, as shown in Fig. 1. For this configuration (3) maintains, whereas (1b) describes a set of five concentric circles in the ξ-η plane. Intersection of these curves gives the energies of the system, in accord with (1c).

B. Density of states

To apply these findings to an infinite array of quantum wells, we note the following. Consider a chain of $Z \geq N$ quantum wells, with each well depth chosen randomly from the following set of N well depths:

$$V_n \propto \rho_n^2 = (n + \tfrac{1}{2})\pi^2 \ , \tag{4a}$$

where the integer n assumes the values

$$0 \leq n \leq N - 1 \ . \tag{4b}$$

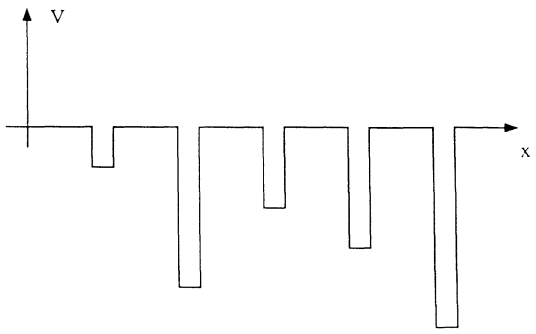

FIG. 1. An array of five quantum wells with randomly distributed depths. In this representation, energies of eigenstates are measured from the top of the well downward to a given level.

Corresponding circles in the ξ-η plane, for the value $N = 11$, superimposed with the transcendental relations (3), are shown in Fig. 2.

From the large numbers' hypothesis, as $Z \to \infty$, the probability of finding a particular well depth V_n approaches $1/N$, so that in this limit it is equally probable to find any of the depths as given by the sequence (4). The number of well depths, N, in any such distribution measures the degree of disorder of the potential array.

In the present work, this disorder parameter assumes the four values $N = 100$, 500, 1500, and 4500. For each value of N, the corresponding interval in energy [recall (1c)] is divided into 150 equally spaced increments, with energy ranging from zero to the ground state of the deepest well in the given array, which is of depth V_{N-1}. Stemming from graphs such as shown in Fig. 2, a histogram of the number of states falling in each interval is computed. Employing a least-squares fit, an assortment of smooth functional forms was applied to this histogram. The polynomial expression

$$D(\varepsilon) = 7.4 - 1.8\varepsilon + 0.50\varepsilon^2 - 0.098\varepsilon^3 \ , \tag{5a}$$

$$D(\varepsilon) = 0, \quad \varepsilon > V_N \ , \tag{5b}$$

$$\varepsilon \equiv 10^4 \eta^2 \tag{5c}$$

consistently proved most accurate. Four examples of this polynomial approximation corresponding to the values $N = 100$, 500, 1500, and 4500 are shown in Fig. 3 and Table I. With these figures at hand, we see that $D(\varepsilon)$ is a more accurate expression of the density of states at larger values of the disorder parameter N. Note also that for each N configuration, the interval over ε increases with N or, equivalently, with the range of well depths. The cutoff in $D(\varepsilon)$ given in (5b) is due to the fact that no energies exist for values in excess of the depth of the Nth well in sequence (4).

Let us denote $D(\varepsilon, N)$ as the density of states for a quantum-well array with disorder N. As noted in the In-

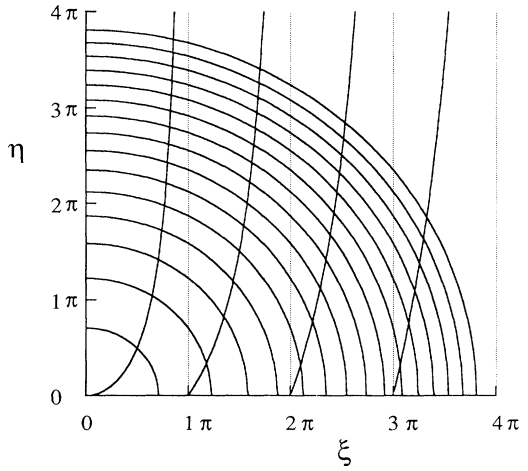

FIG. 2. Characteristic dispersion curves corresponding to the uniform array of potential-well depths of (4a). Energies of the system are given by the intersection of the concentric circles and transcendental curves.

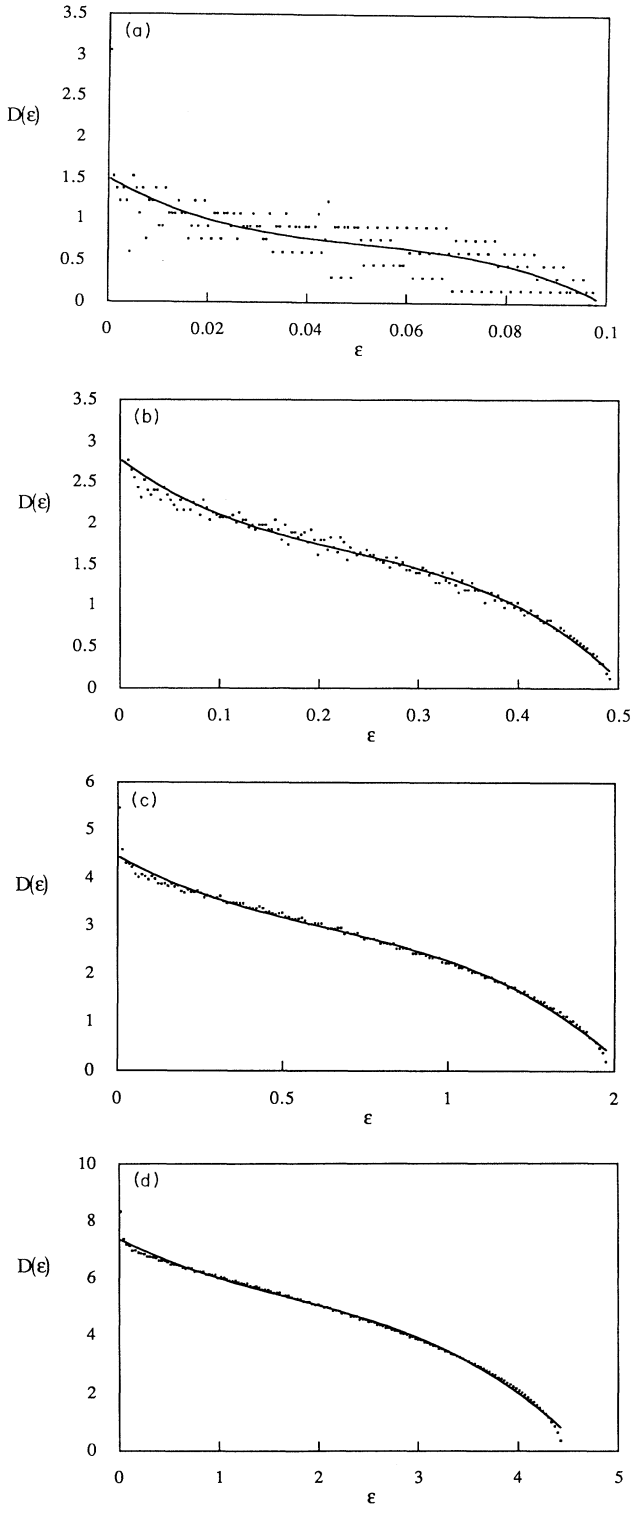

FIG. 3. Fit of the third-order polynomial curve

$$D(\varepsilon)=A_0-A_1\varepsilon+A_2\varepsilon^2-A_3\varepsilon^3$$

to the histogram of energies for $N=$ (a) 100, (b) 500, (c) 1500, and (d) 4500. Values of the coefficients A_i at different N values are given in Table I.

TABLE I. Values of the coefficients A_i at different N values in Fig. 3.

N	A_0	$-A_1$	A_2	$-A_3$
100	1.50	35.3	576	3751
500	2.78	9.05	27.1	39.3
1500	4.45	3.82	3.53	1.88
4500	7.37	1.76	0.500	0.0986

troduction, for each such value of N, $D(\varepsilon,N)$ has a dual interpretation: (a) The ensemble average density of states for a disordered array of N quantum wells, with N varying potential depths. (b) The density of states of an infinite chain of quantum wells, with N varying potential depths randomly distributed over the potential array. For all values of N considered, the related density function exhibits localization of energies about the maximum bound-state energy, $\varepsilon=0$.

C. Density of nearest-neighbor energies

The topic of the density of nearest-neighbor spacing of energies has received much attention in the recent past.[27–30] This problem is returned to for the present configuration. The distribution obtained illustrates strong attraction between eigenvalues and is found to be well approximated by the exponential relation

$$P(s)=6.25\times10^5 e^{-3.82s}, \tag{6}$$

where s represents nearest-neighbor incremental energy spacing and $P(s)$ is its probability density. (For the present situation, $s=\Delta\eta^2$.) The density (6) is plotted in Fig. 4.

As has been found by Berry and Tabor,[24] for quantum systems of dimension greater than 1, with corresponding integrable classical motion whose energy curves in action space are curved, $P(s)$ is roughly Poissonian. Thus the present findings suggest that the Berry-Tabor theorem is valid for one-dimensional motion as well.

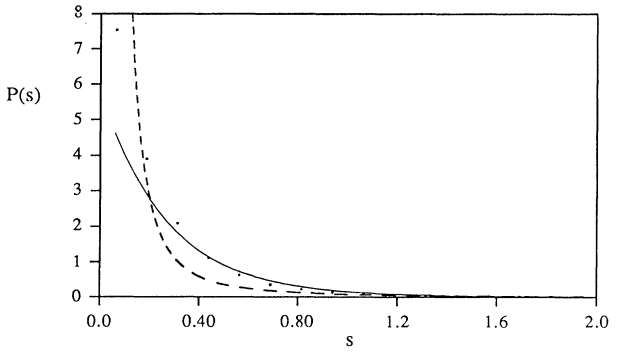

FIG. 4. The density of nearest-neighbor energy spacings, $P(s)$, corresponding to the disorder parameter $N=4500$. The values of $P(s)$ shown have been divided by 10^5. Both power-law (dashed line) and exponential (solid line) fits are shown, from which it is evident that the exponential form better approximates $P(s)$.

III. CONCLUSIONS

To conclude, we have introduced a technique for estimating the smooth component of the density of states of an array of one-dimensional rectangular quantum wells in the weak-coupling limit. The validity of this model was argued on the basis of LCAO results. For the various degrees of disorder considered, the density of states was found to be well approximated by a third-order polynomial. This polynomial fit was noted to grow more accurate with increase in the degree of disorder of the system. The resulting expression for the density of states, (5a), is appropriate to the large-disorder, weak-coupling limit. This result may be considered as a limiting case, in which studies of a disordered array with positive coupling should reduce as the coupling goes to zero. The analysis concludes with a study of the distribution of nearest-neighbor spacings of energies which, for the present configuration, was found to exhibit strong attraction between eigenvalues. This distribution was found to be well represented by an exponential fit, which, as noted, suggests that the Berry-Tabor theorem is valid for one-dimensional motion as well as higher dimensions.

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