# POTENTIALS SUPPORTING POSITIVE-ENERGY EIGENSTATES AND THEIR APPLICATION TO SEMICONDUCTOR HETEROSTRUCTURES

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Herrick has proposed using semiconductor epitaxial heterostructures to create continuum embedded eigenstates (infinitely sharp resonances) of the Wigner-von Neumann type. This paper presents a modification of Herrick's construction rules which should simplify fabrication and improve operation of those heterostructures. The modified procedure has also been generalized to produce for the first time a family of local potentials which simultaneously support two continuum-embedded bound states. Finally, it is pointed out that cases can be generated for which infinitely sharp resonances exist which do not correspond to normalizable bound states.

#### 1. Introduction

Following an original suggestion due to von Neumann and Wigner [1] (corrected subsequently by Simon [2]) many quantum-mechanical examples of local potentials have been constructed which produce positive-energy eigenstates [3, 4]. These eigenstates are embedded in a dense continuum of scattering states of the same symmetry, and they may be regarded as infinitely narrow resonances.

One-dimensional potentials V(x) having this property have invariably exhibited oscillations as  $x \to \pm \infty$ , and in doing so have dropped to zero amplitude no more rapidly than  $|x|^{-1}$ . It is known that potentials with shorter range than  $|x|^{-1}$  cannot produce these states; in those that do, the oscillations create a form of diffractive interference that confers square-integrability on the wavefunction [5].

On account of the oscillations in V(x), these onedimensional examples had been regarded as mathematical curiosities with no direct physical relevance. However, Herrick has recently pointed out [6] that epitaxial GaAs-Al<sub>y</sub>Ga<sub>1-y</sub>As heterostructures might provide a way to construct the V(x) to order, using the fact that band-edge energy varies with composition (y). This suggestion was an outgrowth of detailed experimental observations on one-dimensional quantum states in such devices, for which Dingle has provided a convenient review [7]. Herrick proposed specific structures for production of the positiveenergy states, generalizing a prior mathematical model due to Weidmann [3].

The present paper offers two innovations. The first is largely technical, being concerned with modification of the Weidmann-Herrick models to simplify construction of relevant semiconductor heterostructures. The following section 2 explains this modification. The second innovation involves construction for the first time of potentials that simultaneously support *two* distinct positive-energy eigenstates (section 3). If Herrick's proposal is valid, these two-state potentials could also be produced in semiconductor heterostructure devices.

#### 2. Constant-width layer heterostructures

We consider the x-direction motion of a carrier with effective mass m. As a result of lattice composition variation along this direction, the energy of the relevant band edge will also vary, and may be denoted by V(x). The wavefunction  $\psi(x)$  for carrier motion at energy E along the x direction will be assumed to satisfy the Schrödinger wave equation:

$$\left\{-\frac{1}{2}\frac{d^2}{dx^2} + \frac{m}{\hbar^2}\left[V(x) - E\right]\right\}\psi(x) = 0.$$
 (2.1)

For the cases of principal concern here, lattice composition will approach a fixed value as  $x \to \pm \infty$ , and the zero of energy will be chosen so that V(x) vanishes in these limits.

The Weidmann-Herrick potentials which produce a single localized state at positive energy E, are constant across each of an infinite sequence of intervals. According to Herrick's prescription, these intervals would be fabricated each with a characteristic lattice composition to achieve the desired constant potential. The widths of these intervals vary in a controlled manner across the heterostructure to induce the proper interference effects in  $\psi$ . In all of the examples proposed by Weidmann [3] and by Herrick [6], an infinite number of distinct interval widths is required.

In view of the fact that the semiconductor heterostructures exist essentially in a fixed underlying lattice, it is desirable to have each interval width an integer multiple of a basic length unit (a lattice period). Actually it is possible to have all intervals equal in width, as we now demonstrate.

Our construction is based on the elementary two-layer "module", for which

$$V(x) = V_1$$
 (0 ≤ x < a)  
=  $V_2$  (a ≤ x < 2a), (2.2)

where  $V_1$  and  $V_2$  are suitable constants, and where *a* stands for the common layer width to be used throughout. We shall require that

$$\psi'(0) = \psi'(2a) = 0. \tag{2.3}$$

with a phase change of  $\pi$  between these two endpoints, implying one wavefunction zero.

In each of the two length-*a* intervals  $\psi$  is a simple trigonometric function, so we write

$$\psi(x) = \cos (k_1 x) \qquad (0 \le x \le a)$$
  
=  $A \cos [k_2(x + \delta)] \qquad (a \le x \le 2a).$  (2.4)

Obviously we must have

$$\frac{1}{2}k_1^2 = (m/\hbar^2)(E - V_1), \quad \frac{1}{2}k_2^2 = (m/\hbar^2)(E - V_2). \quad (2.5)$$

Furthermore the phase of  $\psi(2a)$  determines  $\delta$ :

$$k_2\delta = \pi - 2k_2a. \tag{2.6}$$

The condition that  $\psi$  be continuous at x = a provides an expression for the amplitude modulation factor A:

$$A = -\cos(k_1 a) / \cos(k_2 a).$$
(2.7)

We will want 0 < A < 1 so that the module effects a net amplitude decrease in  $\psi$  in going from x = 0 to x = 2a. By placing such modules along the +x axis one after the other, and their mirror images along the -x axis,  $\psi$  can be localized sufficiently to assure square-integrability.

By requiring  $\psi'$  to be continuous at x = a, one finds

$$(k_1a) \tan (k_1a) = -(k_2a) \tan (k_2a).$$
 (2.8)

This equation amounts to a relationship between  $V_1$ and  $V_2$  that must be satisfied in order that  $\psi$  have the postulated form. Thus we are left with a one-parameter family of pairs  $(V_1, V_2)$  out of which the modules may be constructed.

Figure 1 shows plots of numerically calculated  $(V_1, V_2)$  pairs in terms of the reduced values

$$v_j = (ma^2/\hbar^2)V_j$$
 (j = 1,2). (2.9)



Fig. 1. Relation between reduced potentials,  $v_1$  and  $v_2$ , and the amplitude modulation factor  $A(v_1)$ , for the two-layer module discussed in section 2.

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Included as well are the corresponding amplitude factors A. It is worth noting that the most effective amplitude reduction (i.e. smallest A value) occurs when:

$$v_1 = 0.6168, \quad v_2 = -1.6167, \quad A = 0.60899.$$
 (2.10)

In all cases, the energy eigenvalue is

$$E = \pi^2 \hbar^2 / 8ma^2.$$
 (2.11)

Since V(x) must converge to zero at  $\pm\infty$ , formation of a potential supporting a positive energy eigenstate will utilize smaller and smaller values of  $V_1$  and  $V_2$  as these limits are approached. Therefore it is valuable to establish the exact limiting forms of the relationships connecting  $V_1$  to  $V_2$  and to A. By carrying out the necessary series expansions in eqs. (2.7) and (2.8) one finds

$$v_{2} = -v_{1} - (12/\pi^{2})v_{1}^{2} + \mathcal{O}(v_{1}^{3}),$$
  

$$A = 1 - (8/\pi^{2})v_{1} + \mathcal{O}(v_{1}^{2}).$$
(2.12)

Define a modular potential  $V_{\rm m}(x|V_{\rm l})$  as follows:

$$V_{\rm m}(x|V_1) = 0 \qquad (x < 0)$$
  
=  $V_1 \qquad (0 \le x < a)$   
=  $V_2 \qquad (a \le x < 2a)$   
=  $0 \qquad (2a < x)$ , (2.13)

where  $V_2$  is determined by  $V_1$  as above. A symmetrical heterostructure potential V(x) may then be represented as a sum of modular units:

$$V(x) = \sum_{n=0}^{\infty} \left[ V_{\rm m}(x - 2na|V_1^{(n)}) + V_{\rm m}(2na - x|V_1^{(n)}) \right].$$
(2.14)

Wide flexibility exists in choice of the sequence  $V_1^{(0)}$ ,  $V_1^{(1)}$ ,  $V_1^{(2)}$ , ... to produce positive energy eigenstates. However, these quantities *must* converge toward zero no faster than  $n^{-1}$  as  $n \to \infty$ , for otherwise  $\psi$  will not be square-integrable. In terms of the corresponding reduced values  $v_1^{(n)}$  [see eq. (2.9)], one thus demands

$$v_1^{(n)} \sim K/n \quad (n \to \infty), \tag{2.15}$$

where the constant K must be positive. Then it is easy to show from the second of eqs. (2.12) that as  $x \to \pm \infty$ ,

$$\psi(x) \simeq \text{const.} \times |x|^{-8K/\pi^2} \cos{(\pi x/2a)}.$$
 (2.16)

In order that  $\psi^2$  be integrable, it is necessary that the magnitude of the exponent in eq. (2.16) be larger than  $\frac{1}{2}$ . Consequently, rule (2.15) requires

$$K > \pi^2 / 16 = 0.61685 \dots$$
 (2.17)

Whereas the theory of positive-energy eigenstates strictly requires an infinite number of modular units in V(x), eq. (2.14), real heterostructure fabrication would necessarily be limited to a finite number. Consequently, it is important to identify experimentally feasible structures which efficiently approach the behavior of the infinitely extended V(x) with a modest finite number of layers. Thus one seeks a simple arrangement which leads to a narrow resonance behavior, even in the absence of strict wavefunction square-integrability.

The parameters (2.10) are an obvious choice. If V(x) is constructed according to eq. (2.14), with N successive  $V_1^{(n)}$  values corresponding to that optimal choice (i.e. 2N modules), with  $V_1 \equiv 0$  outside this truncated heterostructure region, then  $(0.60899)^N$  becomes the wavefunction amplitude ratio for positions outside the heterostructure, and at its middle. Even for relatively small N (say 30–50), this obviously produces strong resonance confinement of carriers. Additional modules, obeying eq. (2.15), might also be added if experimentally practical.

Experimentally convenient compositions out of which a resonance heterostructure module could be constructed would be  $Al_{0.2}Ga_{0.8}As$ , and GaAs. Conduction electrons have effective mass 0.067  $m_0$  in these lattices. Furthermore, the valence band edge of the former lies 220 meV above that of the latter [7]. Therefore one can use  $Al_{0.2}Ga_{0.8}As$  to provide potential  $V_1$ , and GaAs to provide potential  $V_2$  in the optimum case identified in eqs. (2.10). Assuming linear dependence of band edge energy on composition, the bulk material to be used outside of the sandwich



Fig. 2. Symmetrical heterostructure with a valence-band electron resonance level. Although only 2N = 12 modular units are shown for figure clarity, larger numbers of those units are desirable to sharpen the resonance. Each layer has width 33.98 Å.

region [corresponding to V(x) = 0 above] would have the composition:

$$Al_{0.1448}Ga_{0.8552}As.$$
 (2.18)

From eqs. (2.9) and (2.11), one easily calculates the required layer width *a*, and the resonance energy position *E* [relative to the band edge for composition (2.18)], to have the following values:

$$a = 33.98 \text{ Å}, \quad E = 121.52 \text{ meV}.$$
 (2.19)

The resonance heterostructure is illustrated schematically in fig. 2.

While still utilizing the advantageous reduced parameters (2.10), layer width a and resonance energy E could be varied by employing different layer compositions. Generally, the greater the difference in Al concentrations in adjacent layers, the smaller will aand the larger will E become.

It would be interesting not only to try to observe resonance behavior in the suggested heterostructure, but to look for sharpening of the resonance as the number 2N of modules increases.

#### 3. Potentials with two positive-energy eigenstates

The procedure employed in the preceding section can be extended in such a way that it creates potentials with two positive-energy localized states. In order to do so, we examine a prototypical module with three equal-width layers. Within the three-layer module, the potential will be:

$$V(x) = V_1 \quad (0 \le x < a)$$
  
=  $V_2 \quad (a \le x < 2a)$   
=  $V_3 \quad (2a \le x < 3a).$  (3.1)

As before, the  $V_j$  are constants whose relative magnitudes must be carefully chosen to induce the desired effect.

Let  $\psi$  and  $\Psi$  denote the two positive-energy eigenfunctions, which are square-integrable solutions to the appropriate version of eq. (2.1). We shall require that  $\psi$  and  $\Psi$  respectively increase their phases by  $\pi$  and by  $2\pi$  over the interval  $0 \le x \le 3a$ . Specifically, we can write

$$\psi(x) = \cos (k_1 x) \qquad (0 \le x \le a)$$
  
=  $f \cos [k_2(x + \delta_2)] \qquad (a \le x \le 2a)$   
=  $g \cos [k_3(x + \delta_3)] \qquad (2a \le x \le 3a), \qquad (3.2)$ 

and

$$\Psi(x) = \cos (K_1 x) \qquad (0 \le x \le a)$$
  
=  $F \cos [K_2(x + \Delta_2)] \qquad (a \le x \le 2a)$   
=  $G \cos [K_2(x + \Delta_3)] \qquad (2a \le x \le 3a).$  (3.3)

Triplets  $(V_1, V_2, V_3)$  must be chosen to cause

$$0 < g, G < 1, \tag{3.4}$$

so that successive modules reduce amplitudes for both  $\psi$  and  $\Psi$  as  $|x| \rightarrow \infty$ .

The energies of the states  $\psi$  and  $\Psi$  can be determined by setting  $V_1, V_2$ , and  $V_3$  all equal to zero, and imposing the cited phase increments. Thus one has:

$$E(\psi) = \pi^2 \hbar^2 / 18ma^2, \quad E(\Psi) = 2\pi^2 \hbar^2 / 9ma^2.$$
(3.5)

The wavevectors appearing in eqs. (3.2) and (3.3) for

general  $V_1$ ,  $V_2$ , and  $V_3$  consequently will be (j = 1, 2, 3):

$$k_j = [(\pi^2/9) - 2v_j]^{\frac{1}{2}}/a, \quad K_j = [(4\pi^2/9) - 2v_j]^{\frac{1}{2}}/a, \quad (3.6)$$

where reduced potentials  $v_j$  have been used following the earlier definition (2.9).

The conditions that must be imposed on  $\psi$  and  $\Psi$ are (1) continuity at x = a and x = 2a; (2) continuity of first derivatives at x = a and x = 2a; (3) vanishing of  $\psi'$  and  $\Psi'$  at x = 3a. The resulting equations give, first, expressions for the amplitude modulation factors:

$$g = -\frac{\cos(k_1 a) \cos[k_2(2a + \delta_2)]}{\cos[k_2(a + \delta_2)] \cos(k_3 a)},$$
  

$$G = \frac{\cos(K_1 a) \cos[K_2(2a + \Delta_2)]}{\cos[K_2(a + \Delta_2)] \cos(K_3 a)}.$$
(3.7)

Second, the phase shifts  $\delta_2$  and  $\Delta_2$  may be regarded as determined by:

$$k_{2}(a + \delta_{2}) = \tan^{-1} \left[ \frac{(k_{1}a) \tan(k_{1}a)}{(k_{2}a)} \right],$$

$$K_{2}(a + \Delta_{2}) = \tan^{-1} \left[ \frac{(K_{1}a) \tan(K_{1}a)}{(K_{2}a)} \right].$$
(3.8)

(with due account given to choice of branch for tan<sup>-1</sup>). Third, one has two relations just among the wavevectors:

$$(k_{1}a) \tan (k_{1}a)$$
  
=  $-(k_{2}a) \left[ \frac{(k_{2}a) \tan (k_{2}a) + (k_{3}a) \tan (k_{3}a)}{(k_{2}a) - (k_{3}a) \tan (k_{2}a) \tan (k_{3}a)} \right],$   
(3.9a)

$$= -(K_2a) \left[ \frac{(K_2a)\tan(K_2a) + (K_3a)\tan(K_3a)}{(K_2a) - (K_3a)\tan(K_2a)\tan(K_3a)} \right].$$
(3.9b)

 $(K_1a)$  tan  $(K_1a)$ 

The last pair of eqs. (3.9) constitute two relations among the three quantities  $V_1$ ,  $V_2$ , and  $V_3$ , and can be expected to be satisfied only by a one-parameter family of triplets ( $V_1$ ,  $V_2$ ,  $V_3$ ). Once such a triplet has been found, eqs. (3.8) allow  $\delta_2$  and  $\Delta_2$  to be evaluated. Finally, the modulation factors g and G could then be obtained from eqs. (3.7) and checked against the requirement (3.4) for suitability in production of simultaneous positive-energy localized states.

When  $V_2 < 0$ , we have been unable to find real solutions to the eqs. (3.9). However, such solutions do exist when  $V_2 > 0$ . Fig. 3 shows graphically how this comes about; holding  $v_2$  fixed at  $9.972 \times 10^{-2}$ , the  $(v_1, v_3)$  loci which respectively satisfy the two eqs. (3.9) are plotted and indeed intersect. The points of intersection,

$$(v_1, v_3) = (0.2189, -0.4412),$$
 (3.10a)

$$(v_1, v_3) = (-0.4412, 0.2189),$$
 (3.10b)

form a conjugate pair differing only by interchange of  $v_1$  and  $v_3$ . This interchange merely corresponds to reversing the direction of the module, which is always to be expected as a possibility with the mathematical conditions that have been placed on the problem. For the first intersection point (3.10a), we fortunately find that g and G are acceptable by criterion (3.4):

$$g = 0.6291, \quad G = 0.9121.$$
 (3.11)

The reversed module (3.10b) naturally would replace these last quantities by their reciprocals.

Table I presents numerical results for several cases of the type just given. Just as the information in fig. 1



Fig. 3. Relations between  $v_1$  and  $v_3$  implied by eqs. (3.9), for  $v_2 = 9.972 \times 10^{-2}$ . The curves labelled a and b refer to (3.9a) and (3.9b), respectively.

Table I

Representative parameter sets for three-layer modules, to be used in generation of two simultaneous positive-energy eigenstates.

<i>v</i> <sub>1</sub>	υ2	v <sub>3</sub>	g	G
0	0	0	1	1
0.1771	0.0500	-0.2888	0.7236	0.9304
0.2191	0.1000	-0.4420	0.6282	0.9120
0.2503	0.2000	-0.6945	0.5045	0.9018
0.2552	0.3000	-0.9197	0.4321	0.9093
0.2489	0.4000	-1.1315	0.3754	0.9283
0.2370	0.5000	-1.3336	0.3317	0.9566

can in principle be used to generate a family of potentials with one positive energy state, so can table I (with interpolation) be used for potentials supporting two positive energy states. In place of eq. (2.14) we now have the general modular representation of V(x):

$$V(x) = \sum_{n=0}^{\infty} \left[ V_{3,m}(x - 3na|V_2^{(n)}) - V_{3,m}(3na - x|V_2^{(n)}) \right],$$
(3.12)

where the three-layer module functions,

$$V_{3,m}(x|V_2) = 0 \quad (x < 0)$$
  
=  $V_1 \quad (0 \le x < a)$   
=  $V_2 \quad (a \le x < 2a)$  (3.13)  
=  $V_3 \quad (2a \le x < 3a)$   
=  $0 \quad (3a \le x).$ 

have been indexed according to the  $V_2$  values that they incorporate, with  $V_1$  and  $V_3$  values thereby fixed.

In accord with the preceding case, section 2, an infinite number of modular units would be necessary to produce localized (square-integrable) eigenstates  $\psi$  and  $\Psi$ , with  $(V_1^{(n)}, V_2^{(n)}, V_3^{(n)})$  converging to (0,0,0) as  $n \to \infty$ . Hence we have examined the small- $V_2$  behavior of the dependent quantities  $V_1, V_3, g$ , and G. Detailed analysis is complicated and uninformative, so only the final results will be presented.

In terms of the independent parameter  $v_2$ , one finds the leading-order result:

$$v_1 = Cv_2^{1/2} + O(v_2), \quad v_3 = -Cv_2^{1/2} + O(v_2), \quad (3.14)$$

wherein the numerical constant has the value:

$$C = \left[\frac{32\pi^3\sqrt{3}}{128\pi^2 + 84\pi\sqrt{3} - 135}\right]^{\frac{1}{2}} = 1.041\ 148\ 156\ \dots\ .$$
(3.15)

The existence of fractional powers in eq. (3.14) explains the failure to find real solutions for  $v_2 < 0$ . Modulation factors g and G have the following leading-order terms:

$$g = 1 - (27C/2\pi^2)v_2^{\frac{1}{2}} + \mathcal{O}(v_2),$$
  

$$G = 1 - (27C/8\pi^2)v_2^{\frac{1}{2}} + \mathcal{O}(v_2).$$
(3.16)

As before, the existence of normalizable wavefunctions  $\psi$  and  $\Psi$  requires V(x) to diminish no more rapidly than  $|x|^{-1}$  at infinity. In particular we can suppose the following:

$$v_1^{(n)} \sim CL/n, \quad v_2^{(n)} \sim L^2/n^2, \quad v_3^{(n)} \sim -CL/n \quad (3.17)$$

as  $n \to \infty$ , where L is a positive constant. Using the results in eq. (3.16) it is then straightforward to show that  $\psi$  and  $\Psi$  have these large -|x| asymptotes:

$$\psi(x) \sim \text{const.} \times |x|^{-27CL/2\pi^2} \cos(\pi x/3a),$$
  

$$\Psi(x) \sim \text{const.} \times |x|^{-27CL/8\pi^2} \cos(2\pi x/3a).$$
(3.18)

In order that  $\psi^2$  be integrable it is necessary that

$$L > \pi^2/27C;$$
 (3.19)

however, the demand that  $\Psi^2$  be integrable places a stronger condition on L:

$$L > 4\pi^2/27C. \tag{3.20}$$

## 4. Discussion

By strict periodic repetition of a given module (with two or three layers), the wavefunction is forced to undergo exponential decay with increasing distance, as already noted in section 2. Such exponential waveF. H. Stillinger/Positive-energy eigenstates in semiconductor heterostructures

function decay is symptomatic of an energy in a band gap for the given periodic potential. In the case of three-layer modules in section 3, the energies (3.5) evidently both lie in band gaps since module repetition would cause both  $\psi$  and  $\Psi$  to decay exponentially with distance.

Having selected fixed energies at which normalizable positive-energy states are to be created by nonperiodic potentials of type (2.14) or (3.12), it is obvious that modules of all orders *n* cause wavefunction amplitude reduction precisely by this mechanism of causing those energies at every stage *n* to lie in band gaps. This is so even as  $n \to \infty$  where the component potentials  $V_j^{(n)}$  converge toward zero; the associated band gap widths decrease to zero but have always been arranged just to enclose the selected eigenvalues.

When viewed in this light, the general problem of constructing positive-energy bound states seems to have no limitation on the number of such states that can simultaneously exist with an appropriate local potential V(x). By using our modular approach, each of the energy eigenvalues would lie within band gaps for the associated periodic arrays, and the parametric family of modules would cause these band gaps all to shrink to zero width in the vanishing-potential limit. In order specifically to construct three simultaneous states, a four-layer module offers a simple possible solution.

Inequality (2.17) has been noted as a requirement for square-integrability in the construction of section 2. It is interesting to note as well that if instead

$$0 < K \le \pi^2 / 16,$$
 (4.1)

the wavefunction is not normalizable but still converges to zero as  $|x| \rightarrow \infty$ . This leads to the interesting situation, apparently, of an infinitely sharp resonance behavior at the given energy [eq. (2.11)] not associated with a bound state in the conventional sense. It seems odd that this type of scattering resonance, and its implications for analytic S-matrix theory [8], have not been examined before.

Similar remarks apply to the inequalities (3.19) and (3.20) in connection with construction of the two-state example in section 3. If

$$0 < L \le \pi^2/27C,$$
 (4.2)

neither  $\psi$  nor  $\Psi$  are normalizable bound states, though both represent infinitely sharp resonances. If

$$\pi^2/27C < L \le 4\pi^2/27C, \tag{4.3}$$

then  $\psi$  is a proper bound state while  $\Psi$  still is not.

This distinction between the two types of infinitely sharp resonances is obviously not confined to onedimensional problems, but could in principle appear in non-separable three-dimensional scattering problems as well. In all cases, interesting questions arise about how one could experimentally distinguish the two types.

The calculations presented in sections 2 and 3 employed vanishing derivative boundary conditions at the module endpoints. In principle, equally valid alternative conditions would have been vanishing of the wavefunctions themselves at the endpoints. But at least in the two-layer case of section 2 it turns out that these alternative conditions produce far less efficient carrier confinement; the expression for A corresponding to the second of eqs. (2.12) has the linear  $v_1$  term replaced by a cubic term, thus requiring a much longer-ranged V(x) to assure normalizability.

Finally, it should be noted that continuumembedded bound states have previously been constructed in the presence of electric fields [4]. No doubt such cases could be realized by semiconductor heterostructures along the lines advocated in the present paper. These resonance structures might have useful device applications. They would act as effective carrier-trapping structures only under specific electrical bias, and would lose that trapping ability as bias were changed, removed, or reversed.

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