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# The density of states in the continuous spectrum of one-dimensional systems

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**Abstract.** The change in the density of states introduced by some localized potential $\Delta\rho(E)$ is finite even for infinite systems. We derive some simple analytical formulae for this quantity for three different one-dimensional systems: a finite potential step, a uniform electric field and a flat potential. In each case we relate $\Delta\rho(E)$ to some parameters of the wavefunction. Our analytical expressions for $\Delta\rho(E)$ should be useful in analysing the continuous spectrum of layered microstructures. As an example, we determine $\Delta\rho(E)$ above the symmetric and asymmetric quantum wells.

## 1. Introduction

Various three-dimensional (3D) quantum systems can be described with one-dimensional (1D) models. One important example is radial motion in a spherically symmetric potential [1, 2]. Another class of 1D problems appeared as the effective-mass approximation was applied to layered semiconductor structures [3]. Also surface phenomena were sometimes described with 1D models [4, 5].

A truly continuous spectrum corresponds to an infinite quantum system. The density of states (DOS) in such a spectrum is also infinite. For homogeneous systems it is possible to consider the DOS per unit volume (to make it finite) but in many important cases (linear potential and step potential) the DOS is not linear in the size of the system (see [6] and the discussion therein). A new definition of DOS has been proposed in [6] to avoid these problems. However, the physical meaning of this new DOS is different from the standard DOS and therefore it cannot be used for statistical averaging, calculation of optical properties, etc. Physical quantities (e.g. absorption to the continuum) remain finite even if the DOS is infinite.

In most cases it is not the full DOS of an infinite system which is of interest but its change $\Delta\rho(E)$ introduced by some localized perturbation $V(x)$. This could be the scattering potential (in the radial equation), the quantum-well potential or the double-barrier potential. The unperturbed system could be the flat potential, the linear potential, etc. We have studied $\Delta\rho$ numerically in some important cases [7, 8]. The method consists in evaluating $\Delta\rho$ for a finite system and then going to infinity

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with the size of the system. In this process, $\Delta\rho(E)$ becomes a finite and smooth function of energy. However, it is worthwhile to obtain analytical expressions for $\Delta\rho$ without the necessity for referring to a system of finite size. Such expressions were used by some workers but the only derivation which we found was for the flat-potential case [9]. This derivation was based on the advanced S-matrix formalism developed in [10]. In the present paper we show that the expressions for $\Delta\rho$ can be obtained from the simple analysis of the wavefunctions with and without the perturbing potential. A similar analysis for a spherically symmetric impurity potential leads to the Friedel sum rule or the Fumi theorem for impurities in metals (see, e.g., [2]). The analogue of the Friedel sum rule can also be obtained for the surface problem [5]. In metals the change in DOS for the occupied states (below the Fermi level) gives the electronic charge distribution. In semiconductor heterostructures we consider unoccupied continuum states; they can be populated optically or via tunnelling.

We apply our method to three different cases that have important physical applications:

(i) finite potential step (figure 1(*a*));
(ii) linear potential (homogeneous electric field) (figure 1(*b*));
(iii) flat potential (figure 1(*c*)).

In each case we start from a finite system, evaluate $\Delta\rho$ and relate it to the parameters of the wavefunctions. Finally we increase the system size, obtaining the required expressions for $\Delta\rho$ in terms of the wavefunctions of the infinite system. This last step is simple for cases (i) and (ii) where the spectra are non-degenerate both for the finite and for the infinite systems. Case (iii) is more complicated because the finite system has a non-degenerate spectrum while the infinite system is twofold degenerate. Our method can be applied to other infinite 1D systems. As an illustration we determine $\Delta\rho(E)$ in the continuum above the symmetric and asymmetric quantum wells.

The usual definition of the DOS (for a finite system) involves the sum of $\delta$-functions centred at each energy. Instead, we prefer to define $\rho(E)$ as the inverse of the spacing of the energy levels. This gives a step-like function instead of a Dirac comb; for the infinite system the two definitions are equivalent.

## 2. Finite potential step

We consider the step of height $V_0$ (figure 1(*a*)). This is similar to the surface-potential problems (see [5]). However, the shift in the DOS (and in the charge density) considered in [5] was due to the presence of the surface (compared with the bulk). Here we consider the shift in the DOS introduced by the localized potential perturbing the step in figure 1(*a*). Let us now determine the DOS.

For the energies $E < V_0$ the wavefunction is $A\sin(kx + \Phi_0)$ for $x < 0$ and $B\exp(-\kappa x)$ for $x > 0$. The boundary conditions [11] at $x = 0$ yield

$$B = A\sin\Phi_0 \tag{1}$$

$$\tan\Phi_0 = -k/\kappa. \tag{2}$$

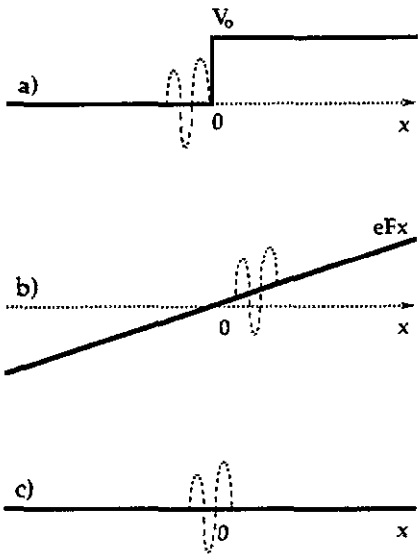


**Figure 1.** The three infinite systems which we consider: ——, potential profiles of the unperturbed systems; – – –, some localized perturbing potentials causing the change $\Delta\rho(E)$ in the DOS.

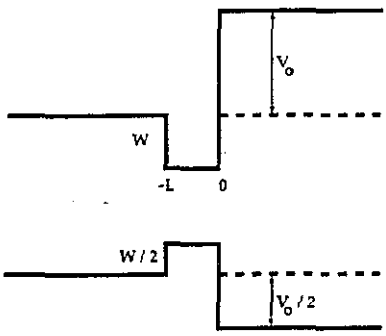


**Figure 2.** Potential profile for the symmetric (- - - -) and asymmetric (——) quantum wells. The band offsets for the holes are taken to be half those for the electrons.

To make the spectrum discrete we add an infinite wall at $x = -L$. This gives the condition for the eigenenergies as

$$kL - \Phi_0(k) = n\pi. \tag{3}$$

The spacing between the subsequent levels is given by

$$\Delta k(L - \mathrm{d}\Phi_0/\mathrm{d}k) = \pi \tag{4}$$

where we assume that $\Phi_0(k)$ is slowly varying with the $\Delta k$ distance, i.e. $\Delta\Phi_0 = (\mathrm{d}\Phi_0/\mathrm{d}k)\,\Delta k$. The DOS of the unperturbed system is

$$\rho_0(k) = 1/\Delta k = (1/\pi)(L + 1/\kappa) \tag{5}$$

where we use equation (2). We can see that indeed the DOS is not proportional to the box size $L$ and that it has a singularity for $E \to V_0$. (For a finite system, $\Phi_0(k)$ is no longer a slowly varying function close to the singularity but by increasing the system size we can get as close to $V_0$ as we wish.) Now we introduce a perturbing potential of the finite range [12], e.g. a quantum well near the step [13]. Outside the potential range the wavefunction can be written as [14] $\tilde{A}\sin(\tilde{k}x + \Phi)$. The infinite well at $x = -L$ leads to the level spacing $\Delta\tilde{k}$ given by

$$\Delta\tilde{k}\,(L - \mathrm{d}\Phi/\mathrm{d}k) = \pi \tag{6}$$

and the change in the DOS

$$\Delta\rho(k) = 1/\Delta\tilde{k} - 1/\Delta k = -(1/\pi)(\mathrm{d}\Phi/\mathrm{d}k + 1/\kappa). \tag{7}$$

This quantity clearly does not depend on $L$ (for large $L$). For the infinite step the second term vanishes. In the energy space,

$$\Delta\rho(E) = \Delta\rho(k)\,\mathrm{d}k/\mathrm{d}E = -(1/\pi)\left(\mathrm{d}\Phi/\mathrm{d}E + 1/\left[2\sqrt{E(V_0 - E)}\right]\right). \tag{8}$$

This means that for the determination of the change in DOS introduced by some localized potential near the finite step it is sufficient to calculate the phase $\Phi(E)$ of the wavefunction $\sin(\bar{k}x + \Phi)$ outside the potential region ($x$ is measured from the step).

### 3. Linear potential

This case corresponds to the homogeneous electric field $F$ (figure 1(*b*)). We put the infinite wall at $x = -L$. In the absence of the perturbation the solution at the energy $E$ is

$$\Psi_E(x) = \mathrm{Ai}(y_x) \tag{9}$$

where

$$y_x = (2meF/\hbar^2)^{1/3}(x - E/eF) \tag{9a}$$

and Ai is the Airy function [15]. It vanishes for $x = -L$ in the finite system. This determines the discrete energy levels. For large $L$, i.e. for $|y_{-L}| \gg 1$ we can use the asymptotic expressions for $\mathrm{Ai}(y)$ (see [15]) and the condition $\Psi_E(-L) = 0$ becomes

$$\sin(\tfrac{2}{3}|y_{-L}|^{3/2} + \tfrac{1}{4}\pi) = 0. \tag{10}$$

Now we turn to the perturbed case; that is at $x > 0$ we have some finite potential $V(x)$, e.g. the quantum well or the superlattice, extending even to $+\infty$. For $x < 0$ the wavefunction is [14]

$$\tilde{\Psi}_{\tilde{E}}(x) = \alpha\,\mathrm{Ai}(\tilde{y}_x) + \beta\,\mathrm{Bi}(\tilde{y}_x) \tag{11}$$

and the discrete energy levels are given by

$$\alpha\,\mathrm{Ai}(\tilde{y}_{-L}) + \beta\,\mathrm{Bi}(\tilde{y}_{-L}) = 0. \tag{12}$$

Now, if we define

$$\tan\Phi = \beta/\alpha \tag{13}$$

and if we use the asymptotic expressions [15] for Ai and Bi we can write equation (12) as

$$\sin(\tfrac{2}{3}|\tilde{y}_{-L}|^{3/2} + \tfrac{1}{4}\pi + \Phi) = 0. \tag{14}$$

For large $L$ we can expand the arguments in equations (10) and (14). For the level spacing $\Delta E$ in the unperturbed case we obtain

$$(2mL/eF\hbar^2)^{1/2}\,\Delta E = \pi \tag{15}$$

and for $\Delta \bar{E}$ in the perturbed case

$$(2mL/eF\hbar^2)^{1/2}\,\Delta \bar{E} + (\mathrm{d}\Phi/\mathrm{d}E)\,\Delta \bar{E} = \pi. \tag{16}$$

The DOS in the linear potential is thus

$$\rho_0(E) = 1/\Delta E = (1/\pi)(2mL/eF\hbar^2)^{1/2} \tag{17}$$

and increases with increasing box size as $\sqrt{L}$. The change in the DOS due to the potential $V(x)$ is

$$\Delta\rho(E) = (1/\pi)(\mathrm{d}\Phi/\mathrm{d}E) \tag{18}$$

or, using equation (13),

$$\Delta\rho(E) = (\alpha\,\mathrm{d}\beta/\mathrm{d}E - \beta\,\mathrm{d}\alpha/\mathrm{d}E)/[\pi(\alpha^2+\beta^2)]. \tag{19}$$

Thus, in both finite and infinite cases the change in DOS is determined by the two coefficients of the wavefunction (11).

#### 4. Flat potential

This case seems to resemble the radial Schrödinger equation for spherically symmetric potentials which has been widely discussed in the context of the scattering theory [1] and in the theory of normal metals [2] (Friedel sum rule). There are, however, important differences between the radial equation and the 1D scattering problem. The radial wavefunctions are defined only for $r > 0$ and are non-degenerate while the 1D case involves doubly degenerate solutions defined for negative and positive arguments. The radial problem bears more resemblance to the potential-step case discussed in section 2.

In the infinite case (in the presence of perturbation) we can use the scattering form of the wavefunction [14]

$$\exp(\mathrm{i}\bar{k}x) + R\exp(-\mathrm{i}\bar{k}x) \qquad T\exp(\mathrm{i}\bar{k}x) \tag{20}$$

and its complex conjugate as two independent solutions. The first function in (20) is the asymptotic solution to the left of the potential region, and the second holds to the right of the potential region. The reflection and transmission coefficients are complex ($R = |R|\exp(\mathrm{i}\phi)$; $T = |T|\exp(\mathrm{i}\psi)$). In the following we shall relate them to the change in DOS introduced by the scattering potential. Here, in order to deal with the finite DOS we put two infinite walls at $x = \pm L/2$.

For the flat-potential case the derivation of $\Delta\rho(E)$ is not as simple as in the two preceding cases. This is because the infinite system is twofold degenerate while the

finite system is non-degenerate. Therefore, two finite-case solutions will contribute to one infinite-case solution.

In the finite case we cannot use the form (20) of the wavefunction because it would not fulfil the boundary conditions at the box edges. Instead, we take the sum of and the difference between (20) and its complex conjugate:

$$\cos(\tilde{k}x) + r_1\cos(\tilde{k}x - \phi_1) \qquad t_1\cos(\tilde{k}x + \psi_1) \tag{21}$$

$$\sin(\tilde{k}x) + r_2\sin(\tilde{k}x - \phi_2) \qquad t_2\sin(\tilde{k}x + \psi_2). \tag{22}$$

The constants $r_i$, $t_i$, $\phi_i$, $\psi_i$ $(i = 1, 2)$ in these two functions can be different for the finite box. Also the energies (i.e. $\tilde{k}$-values) will be different in the finite case. In the infinite case these two solutions will become degenerate. The boundary conditions at $x = L/2$ yield for both solutions

$$\Delta\tilde{k}\,L/2 + \Delta\psi = \pi \tag{23}$$

while in the unperturbed case we simply have $\Delta k\,L/2 = \pi$. The change in DOS due to the perturbing potential is therefore

$$\Delta\rho(k) = (1/\pi)(\mathrm{d}\psi_1/\mathrm{d}k + \mathrm{d}\psi_2/\mathrm{d}k) \tag{24}$$

where we summed the two subdensities corresponding to the two types (21) and (22) of solution. The necessity of treating these two solutions separately stems from the fact that the unperturbed wavefunctions $\sin(kx)$ and $\cos(kx)$ have different phases at $x \simeq 0$ and therefore are affected by the localized potential in very different ways. Our numerical studies of the DOS clearly showed that for the perturbation in the middle of the box we deal with two different smooth subdensities of states. Equation (24) gives us the analytical formula for these subdensities of states.

Before we proceed towards the infinite case it is necessary to take into account some further restrictions on the constants in the wavefunctions (21) and (22). From the boundary conditions at $x = \pm L/2$ we can eliminate $\tilde{k}L/2$, obtaining

$$r_1\sin(\phi_1 - \psi_1) = \sin(\psi_1) \tag{25}$$

$$r_2\sin(\phi_2 - \psi_2) = -\sin(\psi_2). \tag{26}$$

An additional relationship can be obtained from the orthogonality condition for the two solutions, i.e. the term proportional to $L$ should vanish in the overlap integral. This gives

$$[\sin(\phi_1)\sin(\phi_2)]/[\sin(\phi_1 - \psi_1)\sin(\phi_2 - \psi_2)] = t_1t_2. \tag{27}$$

Thus, for large but finite $L$, the solutions (21) and (22) can be written as

$$\alpha\cos(\tilde{k}x - \psi_1) \qquad \cos(\tilde{k}x + \psi_1) \tag{28}$$

$$\sin(\tilde{k}x - \psi_2) \qquad \alpha\sin(\tilde{k}x + \psi_2) \tag{29}$$

where $\alpha = \sin(\phi_1)/[t_1\sin(\phi_1 - \psi_1)]$. For a symmetric perturbation $(V(x) = V(-x))$ we obtain $\alpha = 1$. Therefore, $\alpha$ is the measure of the asymmetry of the system. The

eigenstates in the finite case (outside the potential region) are thus fully characterized by the three constants $\psi_1$, $\psi_2$ and $\alpha$. The allowed values of $\tilde{k}$ are related to the phases by

$$\tilde{k}_1 L/2 + \psi_1(\tilde{k}_1) = (2n-1)\pi/2 \tag{30}$$

for the solution (28) and by

$$\tilde{k}_2 L/2 + \psi_2(\tilde{k}_2) = 2m\pi/2 \tag{31}$$

for the solution (29).

In the limit $L \to \infty$ the wavefunctions (28) and (29) will become degenerate and we can construct the scattering solution (20) from them, i.e.

$$(A_1 + iA_2)\begin{bmatrix} \alpha\cos(\tilde{k}x - \psi_1) \\ \cos(\tilde{k}x + \psi_1) \end{bmatrix} + (B_1 + iB_2)\begin{bmatrix} \sin(\tilde{k}x - \psi_2) \\ \alpha\sin(\tilde{k}x + \psi_2) \end{bmatrix} = \begin{bmatrix} \exp(i\tilde{k}x) + R\exp(-i\tilde{k}x) \\ T\exp(i\tilde{k}x) \end{bmatrix}. \tag{32}$$

The coefficients $A_1$, $A_2$, $B_1$ and $B_2$ can be determined from the above equation in a unique way and we obtain

$$A_1 = [2\alpha/(\alpha^2+1)]\cos(\psi_1) \qquad A_2 = [2\alpha/(\alpha^2+1)]\sin(\psi_1) \tag{33a}$$

$$B_1 = [-2/(\alpha^2+1)]\sin(\psi_2) \qquad B_2 = [2/(\alpha^2+1)]\cos(\psi_2). \tag{33b}$$

We also obtain the expressions for $R$ and $T$ in terms of $\alpha$, $\psi_1$ and $\psi_2$:

$$T = [\alpha/(\alpha^2+1)][\exp(2i\psi_1) + \exp(2i\psi_2)] \tag{34}$$

$$R = [\alpha^2\exp(2i\psi_1) - \exp(2i\psi_2)]/(\alpha^2+1). \tag{35}$$

We can write explicitly the modulus and the phase:

$$|T| = 2|\alpha\cos(\psi_1 - \psi_2)|/(\alpha^2+1) \tag{36}$$

$$\tan\psi = \tan(\psi_1 + \psi_2) \tag{37}$$

$$|R| = \{1 - [4\alpha^2/(\alpha^2+1)^2]\cos^2(\psi_1 - \psi_2)\}^{1/2} \tag{38}$$

$$\tan\phi = [\alpha^2\sin(2\psi_1) - \sin(2\psi_2)]/[\alpha^2\cos(2\psi_1) - \cos(2\psi_2)]. \tag{39}$$

Equation (37) together with equation (24) give us the relationship between $\Delta\rho(k)$ and the phase of transmission, obtained in [9]:

$$\Delta\rho(k) = (1/\pi)(d\psi/dk). \tag{40}$$

Equation (36) relates the maximum transmission to the asymmetry parameter $\alpha$:

$$|T|_{max} = 2|\alpha|/(\alpha^2+1) \tag{41}$$

and equals 1 for a symmetric scattering potential $V(x)$. Equation (38) yields $|R|^2 + |T|^2 = 1$. The phase of the reflection coefficient does not simply relate to $\Delta\rho(k)$ unless $\alpha = 1$ (symmetric $V(x)$). In this case,

$$\tan\phi = -\cot\psi. \tag{42}$$

We can also obtain the transmission coefficient $\overline{T}$ and reflection coefficient $\overline{R}$ in the opposite direction (i.e. for the scattering from right to left) by simply replacing $\alpha \to 1/\alpha$ in equations (34) and (35). This is because the solutions (28) and (29) are non-degenerate and must be proportional to the similar solutions defined for the inverted direction of $x$. We obtain the well known identities

$$\overline{T} = T \tag{43}$$

$$\overline{R} = -\exp[2i(\psi_1 + \psi_2)]\, R^*. \tag{44}$$

Additional relationships between $\Delta\rho(k)$ and $|T(k)|$ can be obtained from the completeness relations for the solutions (28) and (29) (including the possible contribution from the bound states of the potential $V(x)$). A more elegant method consists in studying the analytical properties of $T(k)$ in the plane of complex $k$-values and will be the subject of a separate paper.

## 5. Example: DOS above the quantum well

Let us consider two examples illustrating the formulae derived in the preceding sections. The continuum above the symmetric quantum well (figure 2; $V_0 = 0$) can exhibit some resonances due to interference effects between the two sides of the well. The change in the DOS $\Delta\rho(E)$ can be evaluated from equation (40) with the phase $\psi$ determined from the boundary condition [11] at $x = 0, -L$:

$$\tan(\psi + kL) = \tfrac{1}{2}(k'/k + k/k')\tan(k'L) \tag{45}$$

where $\hbar^2k^2/2m = E$ and $\hbar^2k'^2/2m = E + W$. Using the parameters for the $Al_{0.3}Ga_{0.7}As/GaAs$ quantum well ($m_e = 0.067m_0$, $m_{hh} = 0.45m_0$, $W = 300$ meV and $L = 300$ Å) we obtain $\Delta\rho(E)$ shown as broken curves for electrons in figure 3(*a*) and for heavy holes in figure 3(*b*). Here we assume that the well depth for the holes equals half the well depth for the electrons. The structures in $\Delta\rho(E)$ are more pronounced for the holes but they are weak in both cases. The singularity for $E \to 0$ is of the $1/\sqrt{E}$ type, i.e. $\Delta\rho(k)$ is finite for $k \to 0$.

The second example is the asymmetric quantum well with the right-hand barrier higher than the left-hand barrier by $V_0$ (figure 2). Here we can evaluate $\Delta\rho(E)$ from equation (8), i.e. we treat the system as a perturbed step structure. The phase determined from the boundary conditions is

$$\tan(\phi - kL) = (k/k')[\kappa\sin(k'L) + k'\cos(k'L)]/[k'\sin(k'L) - \kappa\cos(k'L)] \tag{46}$$

where $\hbar^2\kappa^2/2m = V_0 - E$. Using the same parameters as in the previous example and $V_0 = 700$ meV (which corresponds to the $Al_{0.3}Ga_{0.7}As/GaAs/AlAs$ structure) we obtain $\Delta\rho(E)$ shown as full curves in figure 3. Again the resonances for the holes

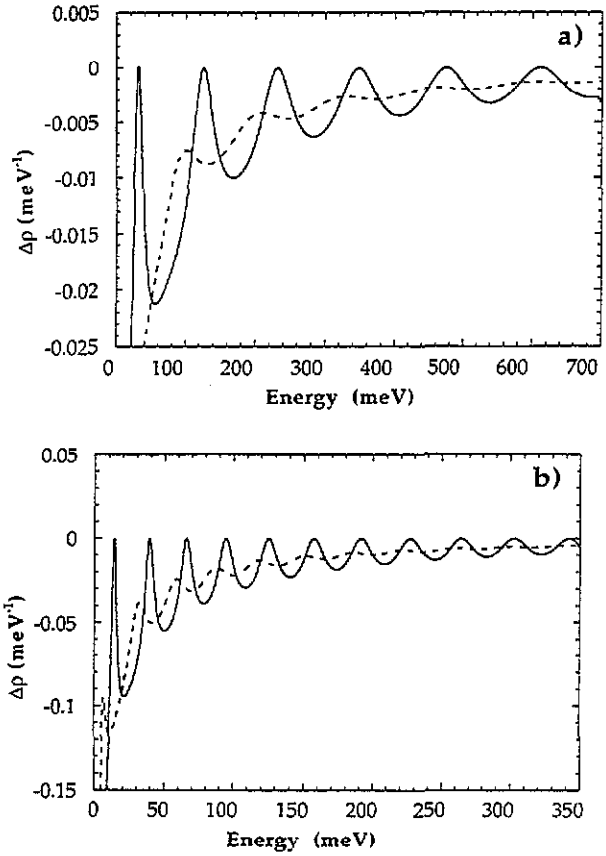


**Figure 3.** Change in the DOS above the wells 300 Å wide of figure 2 ($W$ = 300 meV; $V_0$ = 700 meV) (*a*) for electrons ($m = 0.067m_0$) and (*b*) for heavy holes ($m = 0.45m_0$); ----, $\Delta\rho(E)$ for the symmetric structure; ——, $\Delta\rho(E)$ for the asymmetric structure.

are more pronounced (note the different energy scales in figures 3(*a*) and 3(*b*)). Both for electrons and for holes the resonances are higher and narrower for the asymmetric well. This is because the higher barrier reflects the wavefunction very strongly ($|R| = 1$) compared with the reflection by the symmetric-well barrier and so the interference effects in the continuum are much stronger. In fact the $\Delta\rho(E)$ above the asymmetric quantum well with $V_0 \to \infty$ coincides with the odd subdensity of states (see equation (24)) calculated for the symmetric well of width $2L$. Every wavefunction vanishing for $x = 0$ in the asymmetric well is an odd solution for the symmetric well which is twice as large. The fact that we have no even subdensity makes the resonances more pronounced in the asymmetric-well case.

## 6. Conclusions

We presented a simple method for evaluating $\Delta\rho(E)$ for infinite 1D systems and we applied it to the three potential profiles shown in figure 1. Equations (8), (19) and (40) are the analytical expressions for $\Delta\rho$ in the three cases considered. We used

equations (8) and (40) to compare $\Delta\rho(E)$ in the continuum above the symmetric and asymmetric quantum wells, showing that the asymmetric structure yields much narrower and higher resonances than the symmetric structure does.

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