Optimal band-pass filter for electrons in semiconductor superlattices

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An analytic solution is presented to the problem of designing an anti-reflection coating to be added to an arbitrary periodic superlattice, so as to create an optimal electron band-pass filter.

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I. INTRODUCTION

The propagation of electron waves through layered periodic structures (superlattices) is a problem of continuing interest with practical applications. The basic property of these structures is the appearance of allowed and forbidden energy bands for electrons passing through them. For a superlattice with more than a very few periods, the transmission is almost zero in forbidden bands and shows narrow transmission resonances in the allowed bands.

Recently, a number of authors [1–4] have suggested ways to modify a finite periodic superlattice, so that incident electrons would be fully transmitted over a large part of the entire allowed band, and otherwise reflected. The result would be an energy band-pass filter with a suitably designed superlattice as the active medium. Two ways to modify the basic periodic superlattice were considered: the addition of a cell with new parameters at both ends of the periodic superlattice (an antireflection coating or ARC) by Pacher et al. [1], and the variation of either widths or heights of the barriers of the basic structure itself [2–4]. Here we concentrate on the first method, for which the experiment of Pacher et al. confirmed a significant effect. Moreover, the simplicity of the modification allows us to give a direct and complete solution to the problem.

In the references cited, solutions were obtained numerically and the improvements in transmission properties were presented as recipes, sometimes with little explanation. Further, those solutions are valid only for the square barrier system considered. The problem of modifying an arbitrary initial periodic superlattice to make an energy band-pass filter has not, to our knowledge, been discussed.

In the present paper, we derive general analytical expressions for the parameters of an additional cell (ARC) that should be added at both ends of an *arbitrary* periodic structure in order to achieve optimal transmission within the allowed band. An important aspect of our method is that we concentrate on the envelope of minima of the transmission resonances. This allows us to ensure optimal properties while avoiding the complications associated with the rapidly oscillating amplitudes.

II. GENERAL SOLUTION BY TRANSFER MATRIX METHOD

We consider an arbitrarily shaped real potential cell $v(x)$, defined on $0 < x < d$ and zero otherwise. The potential $v_N(x)$ is defined to be the same potential repeated N times, on the interval $0 < x < Nd$. The corresponding transfer matrices are denoted U and U^N respectively. We denote the transfer matrix of an additional cell $v_a(x)$ on either side of the periodic structure by A. The transfer matrix M for the augmented structure is

$$M = A\, U^N A\,. \tag{1}$$

According to Ref. [5], the transfer matrix A for *any* real potential can be written in terms of its reflection and transmission amplitudes r_a and t_a as

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} 1/t_a & r_a^*/t_a^* \\ r_a/t_a & 1/t_a^* \end{pmatrix}. \tag{2}$$

The matrix U is expressed similarly with replacement of $a \to u$ throughout. Because our potential takes a constant value outside the region where $v(x)$ and $v_a(x)$ are defined, conservation of flux requires that

$$|t_s|^2 + |r_s|^2 = 1\,, \tag{3}$$

where s can be either of the labels u, or a. This makes both $\det U = 1$ and $\det A = 1$.

The N-th power of a unimodular matrix U can be expressed in the form [5]

$$U^N = \frac{\sin N\phi_u}{\sin\phi_u}\, U - \frac{\sin(N-1)\phi_u}{\sin\phi_u}\, 1 \tag{4}$$

where $\cos\phi_u = (u_{11} + u_{22})/2$ defines the Bloch phase associated with the infinitely periodic potential whose unit cell is $v(x)$. Typically, if the number of periods $N > 3$, well defined allowed and forbidden bands for the energy of passing electrons are determined by the properties of the periodic structure. Adding a few additional cells generally changes the transmission properties only inside allowed bands, leaving the transmission through forbidden bands close to zero. (Surface states and isolated states based on defects are an exception to that rule.)

Therefore, the design of an energy band-pass filter proceeds in two steps. First, we select the parameters of a periodic structure with an allowed band in the desired region of energies. We use the lowest allowed band for this purpose, so that all electrons with energies less than its lower boundary E_l will be perfectly reflected. Secondly, we determine the parameters of the additional cells so as to enhance transmission through the allowed band as much as possible.

The Bloch phase is real ($-1 < \cos\phi_u < 1$) in an allowed band. To fix its boundaries we require that

$$\cos\phi_u(E_l) = +1\,; \qquad \cos\phi_u(E_h) = -1 \tag{5}$$

where E_h is the desired upper boundary of the first allowed band. We denote by $E_m = (E_l + E_h)/2$ the energy at the mid-point. (Actually, we can select E_m to be anywhere in the band, but it turns out to be best to be somewhere near the center.)

Next, we choose the parameters of the ARC so that the augmented system will act as a pass-band filter. The transmission through the system can be expressed in terms of the off-diagonal element M_{21} of the total transfer matrix M as

$$|T_N|^2 = \left[1 + |M_{21}|^2\right]^{-1}. \tag{6}$$

Using eq. 2, after some algebra we are able to write

$$|M_{21}|^2 = \left|\alpha^2 - 2\alpha\beta\cos\phi_u + \beta^2\right| \left|\frac{\sin^2(N\phi_u + \delta)}{\sin^2\phi_u}\right|, \tag{7}$$

where the parameters α, β, and δ are simple combinations of elements of the matrices U and A:

$$\begin{aligned} \alpha &= a_{21}(a_{11}u_{11} + a_{22}u_{22}) + a_{11}a_{22}u_{21} + a_{21}^2 u_{12}\,, \\ \beta &= a_{21}(a_{11} + a_{22})\,, \quad \tan\delta = \frac{\beta\sin\phi_u}{\alpha - \beta\cos\phi_u}\,. \end{aligned} \tag{8}$$

When both $v(x)$ and $v_a(x)$ are reflection symmetric, the off-diagonal elements of the matrices U and A are purely imaginary which makes $u_{12} = -u_{21}$ and $a_{12} = -a_{21}$. In this case, (see eq. 2), α and β are pure imaginary, and δ is a real angle. By dropping the factor $\sin^2(N\phi + \delta)$ in eq. 7, we obtain the *envelope of the transmission minima* in allowed bands, which is a curve independent of N:

$$|T_N|^2_{min} = \frac{1}{1 + \left|\alpha^2 - 2\alpha\beta\cos\phi_u + \beta^2\right|/\sin^2\phi_u}\,. \tag{9}$$

By making the envelope reach perfect transmission at $E = E_m$ we obtain the best transmission profile possible, since the first derivative of the transmission minima curve is zero at this point as well. This ensures that deviations of $|T_N|^2$ from unity are minimal except close to the zone boundaries, where $|T_N|^2$ necessarily vanishes.

To obtain such an envelope of minima we must have both $\alpha = 0$ and $\beta = 0$ at the energy E_m. This gives two conditions on the elements of A:

$$\begin{aligned} a_{22} &= -a_{11} \\ \frac{a_{11}}{a_{21}} + \frac{a_{21}}{a_{11}} &= \frac{u_{11} - u_{22}}{u_{21}}\,. \end{aligned} \tag{10}$$

The first line says the additional cell is a Bragg reflector at energy E_m, i.e. $\cos\phi_a(E_m) = \mathrm{Re}[a_{11}] = 0$. Its reflection amplitude $r_a(E_m) = a_{21}/a_{11}$ is purely real at that energy. Then, taking into account eq. 3, we can rewrite the second condition in a physically relevant form as

$$r_a(E_m) = x - \sqrt{x^2 - 1}\,; \quad x = (u_{11} - u_{22})/(2u_{21})\,. \tag{11}$$

When N is large, the oscillations of $|T_N|^2$ are very narrow. Averaging over them, which is appropriate for an incident wave packet, the mean transmission within the allowed band is given by [5]

$$\begin{aligned} |T_N|^2_{av} &= \sqrt{|T_N|^2_{min}} \\ &= \frac{1}{\sqrt{1 + \dfrac{\left|\alpha^2 - 2\alpha\beta\cos\phi_u + \beta^2\right|}{\sin^2\phi_u}}}\,. \end{aligned} \tag{12}$$

This result assumes only that ϕ and δ are varying slowly in comparison with $N\phi_u$.

Finally, we define the average transmissivity τ for electrons passing through the allowed band as

$$\tau = \frac{1}{(E_h - E_l)} \int_{E_l}^{E_h} |T_N|^2 dE\,. \tag{13}$$

τ_{av} is the same quantity, but with integrand $|T_N|^2_{av}$. At least for large N, we expect that $\tau_{av} \to \tau$. Numerical examples (see below) show that this equality holds for N as small as five. Because $|T_N|^2_{av}$ is a smooth curve, the square root of the envelope of minima, it has a clear physical meaning, and τ_{av} is much easier to estimate than is τ.

III. CASE OF DELTA FUNCTIONS

To illustrate our method, we consider an energy band-pass filter consisting of a row of delta-functions of strength C_u and spacing d as the periodic medium. For the unit cell one has (see for example [5])

$$t_u = \frac{k}{k + i\Omega_u} e^{ikd}\,, \quad r_u = \frac{-i\Omega_u}{k + i\Omega_u} e^{ikd}\,, \tag{14}$$

where $k^2 = 2m^* E/\hbar^2$, $\Omega_u = m^* C_u/\hbar^2$, and m^* is the effective mass. The transfer matrix U takes the form

$$U = \begin{pmatrix} (1 + i\Omega_u/k)\, e^{-ikd} & i\Omega_u/k \\ -i\Omega_u/k & (1 - i\Omega_u/k)\, e^{ikd} \end{pmatrix} . \quad (15)$$

The Bloch phase ϕ_u is given by

$$\cos\phi_u(k) = \cos kd + \frac{\Omega_u}{k} \sin kd . \quad (16)$$

The parameters Ω_u and d, are determined by the desired band edges: $\cos\phi_u(k_l) = 1$, and $\cos\phi_u(k_h) = -1$. These lead to

$$\begin{aligned} d &= \pi/k_h \\ \Omega_u &= k_l \tan(k_l d/2) . \end{aligned} \quad (17)$$

If the antireflection cell is a delta potential as well, the cell reflection r_a and transmission t_a amplitudes are fixed by the two conditions (10) with

$$x = \frac{k_m}{\Omega_u} \sin(k_m d) - \cos(k_m d) , \quad k_m^2 = \frac{2m^*}{\hbar^2} E_m . \quad (18)$$

Then, we can find the cell width a and the strength Ω_a using the expressions (14) in which one should replace Ω_u by Ω_a and d by a.

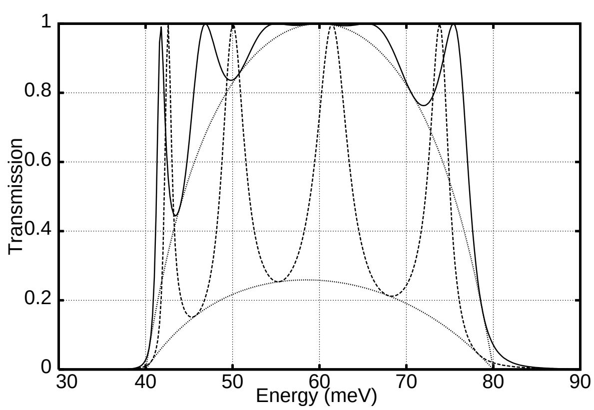

FIG. 1. Transmission probability vs. energy in the first allowed band of a superlattice with $N = 5$ deltas of strength $\Omega_u = 0.55$ nm^{-1} and period $d = 8.14$ nm; dashed line - no additional cells; solid line - there is one additional cell with strength $\Omega_a = 0.23$ nm^{-1} and period $a = 6.52$ nm on each side of the superlattice. Dotted lines are the envelopes of minima.

As a specific example, we place the allowed band at 40 meV$< E <$ 80 meV. Eqs. (17) determine the parameters as $\Omega_u = 0.55$ nm^{-1} and $d = 8.14$ nm; the strength $C_u = \hbar^2 \Omega_u / m^*$ is 590 meV $\cdot$ nm for constant $m^* = 0.071\, m_e$, appropriate to an electron at energy 50 meV above the conduction band edge in $GaAs$. Then, for the additional cell, eqs. (11) with x from eq. (18) gives $r_a(E_m) = 0.57$ and $t_a(E_m) = 0.82i$, which correspond to $\Omega_a = 0.23$ nm^{-1} and $a = 6.52$ nm. The results are shown in Fig. 1. The transmission through the augmented system (solid line) shows a significant increase compared to the transmission for the periodic structure alone (dashed line). The average transmissivity, eq. (13), is $\tau = 0.82$ for the augmented superlattice, double the $\tau = 0.41$ for the initial superlattice. For τ_{av} we find the same transmissivity, within numerical accuracy. This is evidence that the number of periods $N = 5$ can be considered large enough for $|T|^2_{av}$ to be a useful concept. The dotted lines in Fig. 1 show the envelope of transmission minima in both cases.

IV. CASE OF SQUARE BARRIERS

As an application of our result, we consider a band-pass filter based on a square barrier superlattice. The barriers are of height V_u, width d_2, and separated by d_1. The transfer matrix U has elements

$$\begin{aligned} u_{11} &= (\cos\beta d_2 - ic^{(+)} \sin\beta d_2) e^{-ikd_1} = u_{22}^* \\ u_{21} &= -ic^{(-)} \sin(\beta d_2) = u_{12}^* \end{aligned} \quad (19)$$

where $c^{(\pm)} = (k^2 \pm \beta^2)/(2k\beta)$, and $k^2 = 2m^* E/\hbar^2$, $\beta^2 = 2m^*(E - V)/\hbar^2$. The dispersion equation for the Bloch phase ϕ_u is

$$\cos\phi_u = \cos(\beta d_2)\cos(kd_1) - c^{(+)} \sin(\beta d_2)\sin(kd_1) . \quad (20)$$

The allowed band is fixed by the two lowest energy solutions of eq. 5. The reflection amplitude $r_a(E_m)$ of the additional cells is found from eq. 11, where from eq. 19

$$x = \frac{\cos(\beta_m d_2)\sin(k_m d_1) + c_m^{(+)} \sin(\beta_m d_2)\cos(k_m d_1)}{c_m^{(-)} \sin(\beta_m d_2)} \quad (21)$$

with $c_m^{(\pm)}$ evaluated at energy E_m. If we take the additional cell also to be a square barrier, we have the barrier height V_a, the barrier width a_2, and the well width a_1 of $v_a(x)$ to be determined from the expressions for the elements of the matrix A, which has the same form as eq. 19, replacing V, d_1, and d_2 by V_a, a_1, and a_2 respectively.

To be specific, consider a band-pass filter with parameters based on the experiment of Pacher et al. [1]. Their experiment was modelled as a periodic array of $N = 6$ square barriers of height $V = 290$ meV, corresponding to an $Al_{0.3}Ga_{0.7}As$/GaAs superlattice. The barriers were of width $d_2 = 2.54$ nm (9 monolayers of $Al_{0.3}Ga_{0.7}As$) and their wells $d_1 = 6.50$ nm (23 monolayers of GaAs). As before, we use a constant effective mass $m^* = 0.071\, m_e$, appropriate to an energy near the band center. Using eq. 5, the allowed band extends from 49.7 meV$< E <$ 73.2 meV. The lower set of curves in Fig. 2(a) shows the results for this array.

To improve the transmissivity, Pacher et al. [1] took the widths of the barrier and the well of the additional cell to be $a_2 = d_2/2$ and $a_1 = d_1$, keeping the barrier height $V_a = 290$ meV. With this choice, one has an array of six cells, each of which is a resonant tunnelling diode. Their transmission profile is shown by the upper set of lines in Fig. 2(a). Its envelope of minima reaches 100% near the low energy boundary, rather than at the centre of the allowed band. The average transmissivity is $\tau = 0.81$, already a significant improvement over 0.25 for the initial periodic superlattice.

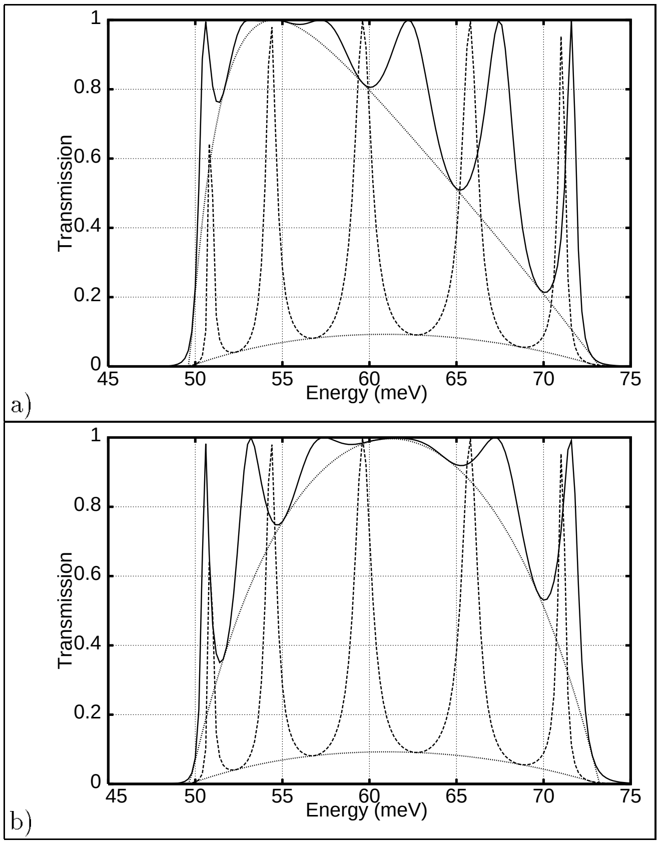

FIG. 2. Transmission probability vs. energy for (a) the device of Pacher et al., and (b) the optimized ARC, as described in text. Dashed lines: without ARC; solid lines, with ARC. The envelope of minima eq. (9) is shown in all cases.

To optimize the ARC, eq. 11 prescribes $r_a(E_m) = 0.73$. For a given barrier height V_a of the additional cell, the well and barrier widths follow from

$$\cos(k_m a_1) = r_a(E_m)\, c^{(+)}_{ma} / c^{(-)}_{ma}$$
$$\cot(\beta_{ma} a_2) = c^{(+)}_{ma}\, \tan(k_m a_1)\,, \qquad (22)$$

where $c^{(\pm)}_{ma} = (k_m^2 \pm \beta^2_{ma})/(2 k_m \beta_{ma})$, and $\beta^2_{ma} = 2m^*(E - V_a)/\hbar^2$.

For $V_a = 300$ meV ($Al_{0.32}Ga_{0.68}As$), the optimal widths are 1.17 nm for the barrier and 5.96 nm for the well. The closest integer number of monolayers is 4 for the barrier, giving $a_2 = 1.13$ nm, and 23 for the well (GaAs), so $a_1 = 5.94$ nm. The results are shown in Fig. 2(b). The transmission profile is improved over that in reference [1], because our envelope of minima is more symmetrically placed, giving a higher transmissivity $\tau = 0.86$. Another solution would be to take $V_a = 153$ meV ($Al_{0.16}Ga_{0.84}As$), giving optimal widths 2.22 nm for the barrier and 5.07 nm for the well. The closest integer number of monolayers is then 8 for the barrier, $a_2 = 2.26$ nm, and 18 for the GaAs well, $a_1 = 5.09$ nm. The results are very similar to the previous case with the same transmissivity $\tau = 0.86$. In all of these examples, $\tau_{av} = \tau$ holds within numerical accuracy.

V. CONCLUSION

Transmission through a superlattice miniband is characterized by a sequence of narrow resonances with $|T|^2$ oscillating between an envelope of minima (see eq. 9), and 100%. When the number of cells is large, the mean transmission probability is given accurately by the square root of that envelope of minima. The design of an efficient filter requires that the envelope of minima touch unity at a point near the centre of the band, and should be as flat as possible in the vicinity.

We have shown how to design an antireflection coating, consisting of a cell placed on either end of the periodic structure, to satisfy this criterion. It must be a Bragg reflector, and must have a reflection coefficient specified by eq. 11. The shape of the potential chosen for the additional cells is arbitrary; all that is necessary is that it provide the required values of $\cos\phi_a$ and $r_a(E_m)$. In our examples we worked with a limited number of parameters so the solution was greatly constrained. Further improvement in the filter properties would require additional derivatives of the envelope of minima to vanish at the chosen energy E_m.

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