The quasiclassical approximation for problems with position dependent mass. The transfer matrix method.

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ABSTRACT

We present the quasiclassical approximation for the 1D-Schrödinger equation with position-dependent mass describing nonhomogeneous semiconductor materials. We develop the transfer matrix method for this approximation and we report the formulae for the solution of five standard problems in quantum mechanics: levels in a well, transmission coefficient of a barrier, quasistationary levels of a well open by one and the two sides and the dispersion relation of a periodical problem. In particular we treat the case when mass and potential have points of finite jump which may be classical turning points.

RESUMEN

Se presenta la aproximación cuasiclásica para los problemas 1D-Schrödinger con masa dependiente de la posición planteados para describir materiales semiconductores inhomogéneos. Se desarrolla el método de la matriz de transferencia para esta aproximación y se reportan fórmulas para las soluciones de cinco problemas importantes de la mecánica cuántica: niveles de un pozo, coeficiente de transmisión de una barrera, niveles cuasiestacionarios de un pozo abierto por uno y ambos extremos y relación de dispersión de un problema periódico. Se trata, en particular, el caso cuando la masa y el potencial tienen puntos de salto finito que pueden ser puntos de retorno clásicos.

1. INTRODUCTION

The 1D problems are one of the most studied in quantum mechanics because of their simplicity and their wide application. The quasiclassical approximation to this kind of problems have provided succes in explaining cualitative aspects of different physical systems. In recent years, with the development of man-made structures as quantum wells and superlattices those fields have been re-examined in many aspects.

In the effective mass approximation, an isolated enough band can be described by a 1D-Schrödinger equation with constant mass [1-2] if the material is homogeneous and with position dependent mass [3-4] if non-homogeneous.

In the present paper we develop the quasiclassical approximation for the 1D-Schrödinger equation with constant and position-dependent mass. Also applying the transfer matriz (TM) method [5] used by the authors for solving this type of problems and [6] specially for the quasiclassical approximation, we study five of the main problems in quantum mechanics; the energy levels of a well, the transmission coefficient of a barrier, the quasistationary levels of a well open by one and the two sides and the dispersion relation of a periodical problem. In particular we emphasize in the case when the mass has points of jump of finite height which may be classical turning points. All these problems are directly related to the study of the energy spectrum, optical and transport properties of layered structures which now can be analized within this approximation.

For completeness, in section 2 we breifly present the quasiclassical approximation for 1D-Schrödinger equation with position-dependent mass; in section 3 we give the main aspects of the TM method particularizing for the case in which the mass has points of jump of finite height. Section 4 is devoted to give the resulting formulae for the above mentioned five problems and to show how some of them become when applying to already known potential profiles in the case of constant mass. Finally we give some conclusions.

2. THE QUASICLASSICAL APPROXIMATION FOR THE 1D-SCHRÖDINGER EQUATION WITH POSITION-DEPENDENT MASS

In [7] the one band Hamiltonians derived in the effective mass theory for nonhomogeneuos systems are summed up in the class:

$$A = \frac{1}{4}\left\{m^{a}(x)\,\hat{p}m^{b}(x)\,\hat{p}m^{c}(x) + m^{c}(x)\,\hat{p}m^{b}(x)\,\hat{p}m^{a}(x)\right\} + V(x) \qquad (1)$$

with a+b+c = −1. In [8] some of the Hamiltonians included in (1) are refused because of difficulties with the solution of already known problems. We shall consider here the case with a=c=0 and b=−1 as the most widelly applied.

In separating variables we obtain the 1D equation of motion with an effective potential given by:

$$V_e(x) = V(x) + \frac{\hbar^2 k_\perp^2}{2m(x)} \quad ; \quad k_\perp^2 = k_y^2 + k_z^2 \tag{2}$$

where V(x) is the original potential considered in the problem.

To solve the equation quasiclassically we follow [9] and considering contributions up to first-order in $\hbar$ we obtain for the solution the expression:

$$F(x) = \sqrt{\frac{m(x)}{k(x)}}\left[A e^{iK(x,a)} + B e^{-iK(x,a)}\right] \tag{3}$$

where we use the notation

$$K(c_2,c_1) = \int_{c_1}^{c_2} |k(x)|\,dx \tag{4}$$

$$k^2(x) \doteq -\kappa^2(x) = 2m(x)\{E-V_e(x)\}/\hbar^2 \tag{5}$$

which we shall use throughout the paper. In (4) c_1 and c_2 are any arbitrary points In (3) "a" in K(x,a) is any fixed point.

Demanding the first-order term in $\hbar$ to the smaller than the zeroth-order term in the power series of the action of the system we obtain the applicability condition for the approximation which is:

$$\left|\frac{1}{m(x)}\frac{d}{dx}\left[\frac{m(x)\lambda(x)}{2}\right]\right| \ll 1 \tag{6}$$

where

$$\lambda(x) = (2\pi)/k(x) \tag{7}$$

Equation (6) reduces to the usually obtained [9] by making m(x)=constant.

To obtain the connection rules for the wave function around a turning point assuming well behaved potential profile and mass distribution, we have to solve the equation for F(x) in the neighborhood of the turning point x=d. Taking the linear approximation for the square of the quasi-wave vector given in (5) it can be shown that the equation obtained can be reduced to an Airy's [10] one. This gives the same connection rules already known, valid for the constant mass problems, provided that the potential profile and mass distribution are slowly varying functions in the neighborhood of the turning point x=d, and the condition:

$$\left|\frac{1}{m(d)}\left[\frac{m'(d)}{m(d)}\right]^3\right| < \left|\frac{V_e'(d)}{\hbar^2}\right| \tag{8}$$

to be satisfied. This condition is obtained in demanding that the interval corresponding to the Airy functions around x=d overlaps the regions where the quasiclassical solutions are valid.

There are other cases of interest among which we have: a) The potential and mass functions have a jump of finite height in a turning point; b) the potential has a jump of finite height in a turning point and the mass is continuous at it (specially here we include the case m=cte.) and c) the potential profile and mass distribution have a jump of finite height at a point which is not a turning point. In all these cases the corresponding quasiclassical solutions are valid up to this point at each side of it and there is unnecesary approximate connection rules. But you have to demand continuity of the current density in crossing this point. This lead us to satisfy the conditions:

$$F(d-) = F(d+)$$
$$\frac{1}{m(d-)} F'(d-) = \frac{1}{m(d+)} F'(d+) \tag{9}$$

(9) will introduce some differences in the corresponding TM as will be seen in the next section.

3. TM FORMALISM FOR THE QUASICLASSICAL SOLUTION

Knowing the form of the solution in a region, it can be constructed the TM by forming a canonical basis [5 and reference 2 therein], for $x=x_0$, and with it the TM.

In [6] we give the results obtained in the case of well behaved mass and potential functions when the points x and x_0 (in between which we make the transfering) lay in the same classically allowed region. We shall use the following notation in further formulae, as done in [6]:

$$y_{11}(c_2,c_1) = \sqrt{\left|\frac{k(c_1)m(c_2)}{k(c_2)m(c_1)}\right|} \qquad y_{22}(c_2,c_1) = \sqrt{\left|\frac{k(c_2)m(c_2)}{k(c_1)m(c_1)}\right|}$$
$$y_{12}(c_2,c_1) = \sqrt{\left|\frac{m(c_2)}{m(c_1)k(c_2)k(c_1)}\right|} \qquad y_{21}(c_2,c_1) = \sqrt{\left|\frac{m(c_2)k(c_2)k(c_1)}{m(c_1)}\right|} \tag{10}$$

here c_2 and c_1 are any arbitrary points.

We report here the matrix elements of the TM corresponding to x and x_0 in the same classically allowed region when there is a point $x=x_r$ where the mass has a jump of finite height in between them. In $x=x_r$ we must satisfy conditions (9), which in matrix form are written as:

$$C(x_r) = \begin{bmatrix} 1 & 0 \\ 0 & \frac{m(x_r+)}{m(x_r-)} \end{bmatrix} \tag{11}$$

Then the TM considered is:

$$M(x,x_0) = M(x,x_r)C(x_r)M(x_r,x_0)$$

where the matrix elements are:

$$\begin{aligned}
M_{11}(x,x_0) &= y_{11}(x,x_0)\{\gamma(x_r)c_1\cos_1-(1/\gamma(x_r))s_1\sin_1\} \\
M_{12}(x,x_0) &= y_{12}(x,x_0)\{\gamma(x_r)s_1\cos_1+(1/\gamma(x_r))c_1\sin_1\} \\
M_{21}(x,x_0) &= y_{21}(x,x_0)\{\gamma(x_r)c_1\sin_1-(1/\gamma(x_r))s_1\cos_1\} \\
M_{22}(x,x_0) &= y_{22}(x,x_0)\{\gamma(x_r)s_1\sin_1+(1/\gamma(x_r))c_1\cos_1\}
\end{aligned} \qquad (12)$$

where:

$$\gamma(x_r) = \left[\frac{-m(x_r-)k(x_r-)}{-m(x_r+)k(x_r+)}\right]^{\frac{1}{2}}$$

$c_1=\cos(K(x_r,x_0))$; $s_1=\sin(K(x_r,x_0))$; $\cos_1=\cos(K(x,x_r))$ and $\sin_1=\sin(K(x,x_r))$

When one makes $m(x_r+)=m(x_r-)$, then (12) reduces to the TM reported in [6].

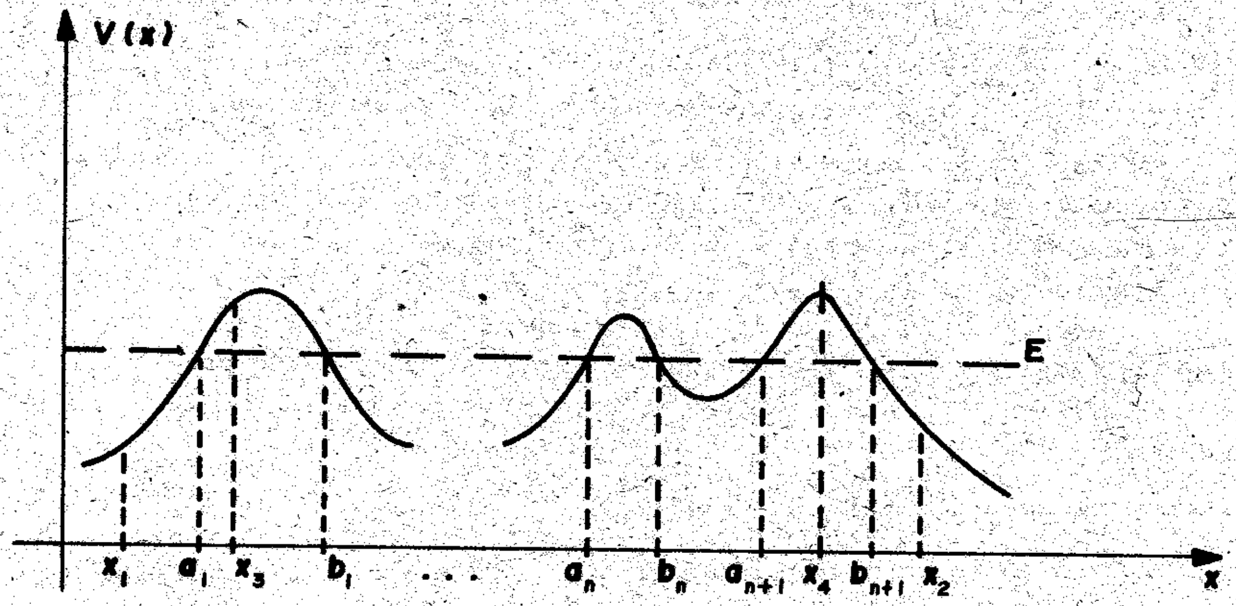

Figure 1. Model of potential (well behaved case) considered in the article, a and b, are turning points and x, are intermediate points

By direct multiplication it can be shown that in any of the cases we have considered, the TM corresponding to transfer from the points depicted in figura 1 can be written as:

$$M_{ij}(x_2,x_1) = y_{ij}\left\{p\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix}e^{i(K_2+K_1)} + q\begin{pmatrix}1 & -i\\ -i & -1\end{pmatrix} e^{-i(K_2-K_1)} + c.c.\right\}_{ij} \qquad (13)$$

$$M_{ij}(x_4,x_3) = y_{ij}\left\{w\begin{pmatrix}1 & 1\\ i & 1\end{pmatrix}e^{K_4+K_3} + u\begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix}e^{(K_4-K_3)} + v\begin{pmatrix}1 & 1\\ -1 & -1\end{pmatrix} e^{-(K_4-K_3)} + \right.$$

$$\left. + t\begin{pmatrix}1 & -1\\ -1 & i\end{pmatrix} e^{-(K_4+K_3)}\right\}_{ij} \qquad (14)$$

$$M_{ij}(x_4,x_1) = y_{ij}\left\{d\begin{pmatrix}1 & -1\\ -1 & i\end{pmatrix}e^{(-K_4+iK_1)} + f\begin{pmatrix}1 & -i\\ 1 & -i\end{pmatrix}e^{(K_4+iK_1)} + c.c.\right\}_{ij} \qquad (15)$$

and

$$K_2=K(x_2,b_{N+1});\quad K_1=K(a_1,x_1);\quad K_3=K(b_1,x_3);\quad K_4=K(x_4,a_{N+1}) \qquad (16)$$

Here y_{ij} are given by (10) and evaluated at the same arguments than M_{ij} where $i,j=1,2$ and c.c. means the corresponding complex conjugate terms.

These expressions represent the general form of the TM in terms of a few parameters (p and q when transfering between points in classically allowed regions; t, u, v and w when transfering between classically forbidden regions and d, f when transfering between points at different kind of regions) which obviously will change in each case. The central point of these forms are the separation attained between the properties of the barrier or well and the variable extreme intervals ((x_1,a_1), for example).

Also we have the following relations:

$$4\{|p|^2 - |q|^2\} = 1 \qquad (17a)$$

$$4\{tw - uv\} = 1 \qquad (17b)$$

$$4i\{df^* - df^*\} = 1 \qquad (17c)$$

which assures the property $\det\{M(c_2,c_1)\} = (m(c_2)/m(c_1))$[11].

In [6] we report the relations between the parameters p, q, t, u, v, w, d and f (valid for the cases of weel behaved potential and mass [6] and the ones treated here). Also we give there the recurrence relations for these parameters which permit to obtain their form for any number of barriers (wells) in terms of the corresponding parameters of one barrier (well), not given here for brevity.

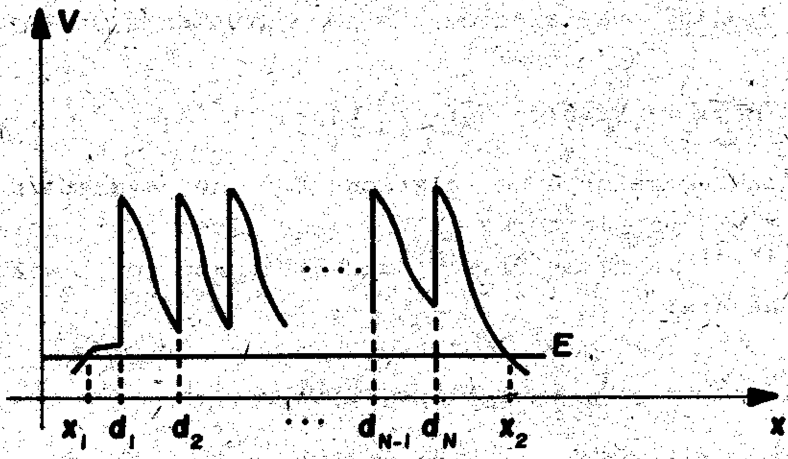

Figure 2. Model of potential with points of jump of finite height (barrier case). d_j are the point of jump. E is the energy considered

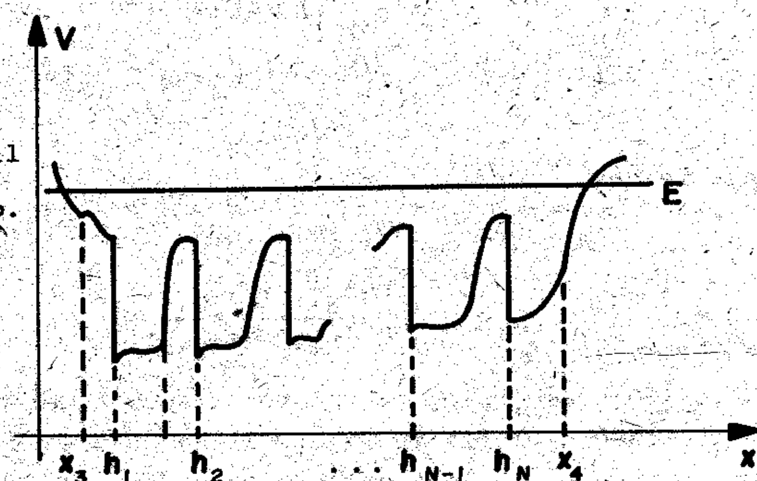

Figure 3. Model of potential with points of jump of finite height (well case). hj are the points of jump. E is the energy considered

In addition, when the mass or potential have points of jump of finite height, one may have situations like the ones depicted in figures 2 and 3. By complete induction procedure it can be proved that the TM in these cases can be written as:

$$M_{ij}(x_2,x_1) = y_{ij}\left\{\alpha\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix}e^{i(K_a+K_b)} + \beta\begin{pmatrix}1 & i\\ i & -1\end{pmatrix}e^{i(K_a-K_b)} + c.c.\right\}_{ij} \qquad (18)$$

$$M_{ij}(x_4,x_3) = y_{ij}\left\{\theta\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}e^{K_c+K_d} + \Omega\begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix}e^{(K_c-K_d)} + \lambda\begin{pmatrix}1 & 1\\ -1 & -1\end{pmatrix}e^{-(K_c-K_d)} + \right.$$

$$\left. + \mu\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}e^{-(K_c+K_d)}\right\}_{ij} \qquad (19)$$

where the y_{ij}'s are given by (10) evaluated at the same arguments of the M_{ij} and:

$$K_a=K(x_2,d_N);\ K_b=K(d_1,x_1);\ K_c=K(x_4,h_N);\ K_d=K(h_1,x_3)$$

Also it is easy to obtain the recurrence relations for the parameters corresponding to N+1 points of jump in terms of the ones given for N points of jump (i.e. $\alpha^{(N+1)}$ and $\beta^{(N+1)}$ in terms of $\alpha^{(N)}$ and $\beta^{(N)}$, and so on with the others). The expressions are:

$$\begin{aligned}
\alpha^{(N+1)} &= A_1\alpha^{(N)}e^{ik(d_{N+1},d_N)}+B_1(\beta^{(N)})^*e^{-ik(d_{N+1},d_N)}\\
\beta^{(N+1)} &= A_1\beta^{(N)}e^{ik(d_{N+1},d_N)}+B_1(\alpha^{(N)})^*e^{-ik(d_{N+1},d_N)}\\
\theta^{(N+1)} &= A_1\theta^{(N)}e^{k(h_{N+1},h_N)}+B_1\lambda^{(N)}e^{-k(h_{N+1},h_N)}\\
\Omega^{(N+1)} &= A_1\Omega^{(N)}e^{k(h_{N+1},h_N)}+B_1\mu^{(N)}e^{-k(h_{N+1},h_N)}\\
\lambda^{(N+1)} &= A_1\theta^{(N)}e^{k(h_{N+1},h_N)}+B_1\lambda^{(N)}e^{-k(h_{N+1},h_N)}\\
\mu^{(N+1)} &= B_1\Omega^{(N)}e^{k(h_{N+1},h_N)}+A_1\mu^{(N)}e^{-k(h_{N+1},h_N)}
\end{aligned} \tag{20}$$

here we have named:

$$A_1 = (1/2)[q+(1/q)];\qquad B_1 = (1/2)[q-(1/q)]$$

$$q = \left|\frac{m(l_{N+1}-)k(l_{N+1}+)}{m(l_{N+1}+)k(l_{N+1}-)}\right|^{\frac{1}{2}}$$

where l=d,h according to the formula considered, and we use modulus because in the case depicted in figure 2 the quasiwave vectors are imaginary. Notice that in the integrals of the form (4) the limits are from the last point of jump to the one added in each case.

We remark that in (20) we explicitly declared the number of points of jump we are dealing with, but in (18) and (19) we omit it and these expressions are general for any points of jump.

In particular, for the case of one point of jump we have:

$$\alpha = q+(1/q)\qquad \beta = q-(1/q) \tag{21}$$

$$\theta = \mu = q+(1/q)\qquad \Omega = \lambda = q-(1/q) \tag{22}$$

We omit, in order to make this paper not too long, the results of parameters p and q when we have a barrier and w, u, v and t when a well with one turning point of jump and for well behaved potential and mass (the last one already reported in [6]), but they are easily obtainable by matrix multiplication.

4. FORMULAE FOR THE STANDARD PROBLEMS

Having the general form of the TM for each type of region considered, we may give the formulae for the standard problems already mentioned for a wide class of potential profiles and mass distributions. We shall study the following problems:

i) Transmission coefficient of the (N+1) barriers between the points a_1 and b_{N+1}.

ii) Energy levels of stationary states of the N wells between the points b_1 and a_{N+1} (considering that the extreme barriers in figure 1 are impervious).

iii) Energy levels of quasistationary states of the N wells potential open by one side (considering that one of the extreme barriers is non-penetrable).

iv) Energy levels of quasistationary states of the N well potential open by the two sides.

v) Energy bands of a periodical potential with unit cell of lenght "L" and with N wells at the energy considered.

In order to obtain the formula for problem i) we take an incident wave comming from $-\infty$ and calculate the fraction of the current density that arrives to $+\infty$. The transmission coefficient is then

$$T = \frac{1}{4|p|^2} \qquad (23)$$

Problem ii) is considered by imposing the solution to be bounded at $\mp\infty$. We obtain as the transcendental equation for the energy levels the following:

$$w = 0 \qquad (24)$$

If we consider the barrier open at its left side and impossing the solution to be bounded at $+\infty$ and an outcoming wave in $x<a_1$, we have the following transcendental equation for the complex energy of the quasistationary state:

$$f^* = 0 \qquad (25)$$

For the problem iv) we impose that at both sides we have only outcoming waves, and we obtain

$$p^* = 0 \qquad (26)$$

(In using (25) and (26) we must be careful: the energy must be treated as a real number in writing these equations for particular cases, but we search for their complex roots.).

The bands of a periodical problem are obtained in diagonalizing the TM of the unit cell $M(x+L,x)$ [2,3]. Here we shall consider the cases of well behaved potential profiles and mass distributions. For energies greater than the maximum of the potential, taking the TM corresponding to an allowed region reported in [6] with $x_2=x_1+L$, it can be shown that the equation for determining the energy bands is:

$$K(x_1+L,x_1) = QL+2n\pi \quad \text{n is an integer} \tag{27}$$

where Q is the wave vector of the periodical problem. This dispersion relation implies an effective mass exactly equal to the classical one for constant mass, and its generalization when the mass is position-dependent [12].

For energies smaller than the maximum of the potential, simple expressions may be obtained in terms of the parameters p, t, etcetera (we may choose the unit cell in order to have a barrier or a well). In this case the effective mass that can be derived in this approximation differs to much from the classical one.

We remark that all formulae (23)-(27) are valid for both constant and position-dependent mass including potential profiles and mass distributions with points of jump of finite height. The main changes among them for different cases are the explicit form of the parameters in which terms we write the TM. (i.e. p, q, w, etcetera).

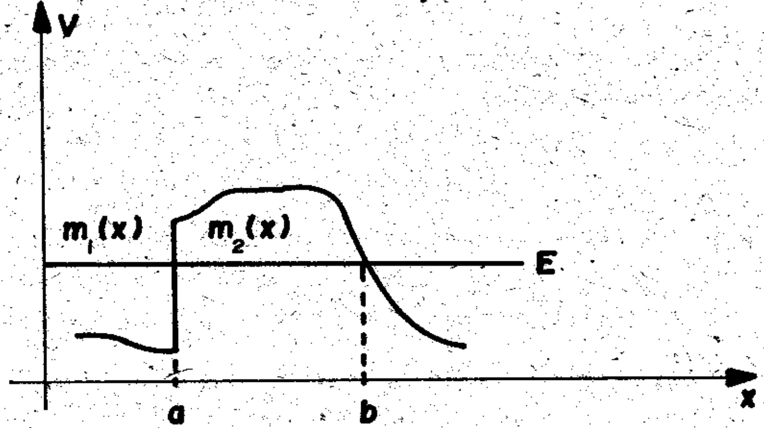

Figura 4. Model of potential of one barrier with one point of jump. Here it is supose that $m(x)$ is $m_1(x)$ for $x<a$ and $m_2(x)$ for $x>a$, different in general

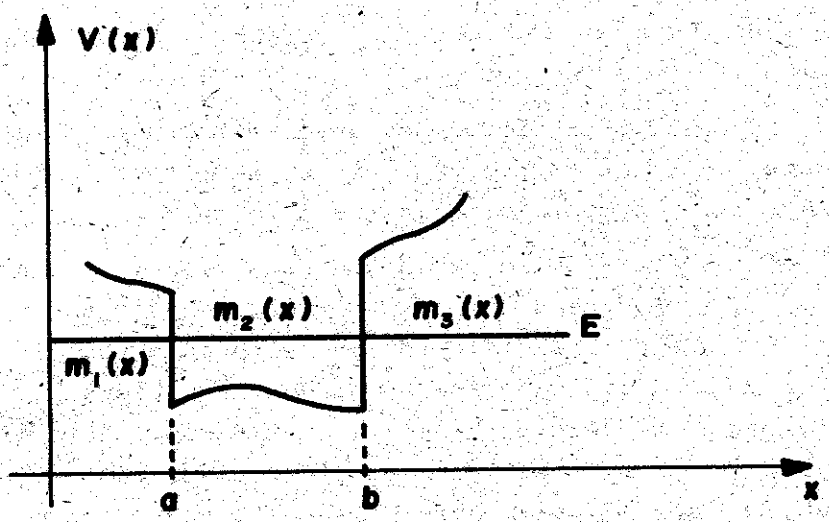

Figure 5. Model of potential of one well with two turning points of jump of finite height. m(x) has three laws (different in principle) in depending on the region.

As examples of the application of the obtained results to particular examples for position-dependent mass we have:

For the barrier shown in figure 4 the transmission coefficient is:

$$T = \frac{4}{\left\{\left[\frac{m_1(a)\xi(a)}{m_2(a)k(a)} + \frac{m_2(a)k(a)}{m_1(a)\xi(a)}\right]\cosh\{2K(b,a)+\ln 2\}+2\right\}} \qquad (28)$$

which reduces to the known result [13] when m(x)=constant.

For the well shown in figure 5 we obtain for the levels the equation:

$$\tan(K(b,a)) = \frac{m_2(b)m_1(a)k_2(a)\xi_2(b)+m_3(b)m_2(a)k_2(b)\xi_1(a)}{m_3(b)m_1(a)k_2(a)k_2(b)-m_2(b)m_2(a)\xi_1(a)\xi_2(b)} \qquad (29)$$

which reduces, for constant mass, to a result easilly obtainable by the standard WKB method.

Here in (28)-(29) we have used the notation declared in (5).

5. CONCLUSIONS

We have developed the quasiclassical approximation for the class of Hamiltonians proposed to describe nonhomogeneous systems. The solution is the same for all of them because the term which make different one Hamiltonian fron another give contributions of order $\hbar^2$ in the power series of the action, not considered in this approximation.

The connection rules we obtain for position-dependent mass are the same given for constant mass when the potential profile and mass distribution are well behaved functions and conditions (9) must be considered when the mass has jumps of finite height.

The main influence of position-dependent mass in this approximation comes from the fact that in $K(c_2,c_1)$ we now have the dependence of mass and potential with the coordinate in the integrand.

We obtained the form of the TM in the quasiclassical approximation for constant and position-dependent mass for well behaved and specially for potential profiles and mass distributions with jumps of finite height. These results in addition with the recurrence relations and formulae (23)-(27) allows us to consider analytical and computational solutions of real multiple barrier systems in an easy and algorithmical way. To do so we start with the set of parameters of a well, or a barrier, etcetera (i.e. p and q; or w, t, u, w, etcetera), in each case. We apply iterativelly the recurrence relations given in [6] which are valid in any case with little changes. These changes become from the relations of α,β, etcetera with parameters (p and q, or w, t, u and v, etcetera). When we have only points of jump, not been turning points, we apply iterativelly (20). In this way we obtain the corresponding parameters of the whole problem we are studying. Applying now (23)-(27), valid in any case considered, we solve the problem we are dealing with.

Finally we report formulae for particular cases of barriers and wells with position-dependent mass, already known to the case of constant mass.

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