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R. Perez-Alvarez

H. Rodriguez-Coppola

V.R. Velasco

and

F. Garcia-Moliner

INTERNATIONAL ATOMIC ENERGY AGENCY

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# MATCHING WITH TRANSFER MATRICES *

R. Pérez-Alvarez **
International Centre for Theoretical Physics, Trieste, Italy,

H. Rodriguez-Coppola
Departamento de Fisica Teórica, Universidad de la Habana,
San Lázaro y L, Habana, Cuba,

V.R. Velasco † and F. Garcia-Moliner †
International Centre for Theoretical Physics, Trieste, Italy.

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** Permanent address: Departamento de Fisica Teórica, Universidad de la Habana, San Lázaro y L, Habana, Cuba.

† Permanent address: Instituto de Ciencia de Materiales, CSIC, Serrano 123, 28006 Madrid, Spain.

## Abstract

An ABC configuration - which corresponds to various systems of physical interest, such as a barrier or a quantum well - is studied by combining a surface Green function matching analysis of the entire system with a description of the intermediate (B) region in terms of a transfer matrix in the sense of Mora et al. (1985). This hybrid approach proves very useful when it is very difficult to construct the corresponding Green function $G_B$. An application is made to the calculation of quantised subband levels in a parabolic quantum well. Further possibilities of extension of this approach are pointed out.

## 1. Introduction

The matching problem for two continuous media meeting at an interface can be studied by means of a Surface Green Function Matching (SGFM) analysis involving the Green functions of the constituent media (García-Moliner and Rubio, 1971; García-Moliner, 1977; García-Moliner and Flores, 1979; Velicky and Bartos, 1971; Inglesfield, 1971). This formalism was first introduced (García-Moliner and Rubio, 1969) to study electronic surface states but it can equally be used to study, say, elastic surface or interface states (Velasco and García-Moliner, 1977,1979,1980), viscoelastic waves in solid-fluid or fluid-fluid interfaces (Platero et al., 1981; Velasco and Navascués, 1986), piezoelectric (Velasco, 1983; Velasco and García-Moliner, 1984) or magnetoelastic (Velasco, 1985; Velasco and García-Moliner, 1985) surface or interface waves or, indeed, any matching problem described by a second order differential equation (García-Moliner, 1977). This formalism has been extended to situations of physical interest involving the simultaneous matching at different coupled interfaces, such as a quantum well or a superlattice (García-Moliner and Velasco, 1986) and has been used to study elastic (Brito et al., 1987) and piezoelectric (Fernández et al., 1987) superlattices, as well as the Stark shift of exciton peak in quantum wells in an external electric field (Glasser and García-Moliner, 1987).

Another possible approach to these problems can be set up based on the concept of *transfer matrix* (TM). This has been used in practice essentially for the Schrödinger equation, i.e., electronic states. This term is given different names in the literature. If



one writes down the form of the wavefunction as a combination of some basis functions - often two plane waves of the same energy running in opposite directions - then the TM is defined (James, 1949; Strandberg, 1982) so that it tranfers the coefficients of this combination from one point to another. There is a different concept of TM, described in Section 3, which transfers the wavefunction itself and its derivative with respect to one coordinate, from one point to another. A preliminary account of this TM was given by Smith (1961) for the case of constant potential. More generally, the mathematical properties of this TM have been studied in detail by Mora et al. (1985) with emphasis again on the Schrödinger equation, although the formal theory is equally valid for any linear second order differential equation or, else, for a set of coupled, linear, first order differential equations. This formalism has also been used to study electronic states in superlattices (de Dios Leyva et al., 1986).

Now, the GF and the TM approaches appear to be unrelated. In fact the two concepts have an inherent difference. The TM makes no reference to boundary conditions while a Green function (GF) is not completely defined until these are specified.

The purpose of this paper is to study the relationship between these two approaches and to turn this into a practical scheme for doing calculations based on a hybrid approach which uses the advantages of either side as convenience advises.

The emphasis is concentrated on an A-B-C configuration where mainly B is 'difficult', meaning for instance that there is no easy way to evaluate the corresponding GF, i.e. $G_B$. While this is not the only configuration which can be studied in the way presently to be described, it does correspond to many situations of physical

interest in which B is some transition region between two perfect media A and C. E.g., B can be a selfconsistent surface or interface potential, or a barrier or well of a complicated shape.

The mathematical elements of the connection between GF and TM are given in Sections 2 and 3, the methodology of the hybrid method is presented in Section 4 and a practical application is given in Section 5.

## 2. The definition of extended pseudomedia in the matching problem.

Firstly consider a one interface problem. Medium A on the left ($z\leq 0$) is matched to medium B on the right ($z\geq 0$). Let M indicate one of the two domains and $\bar{M}$ the other one.

The basic SGFM formulae are

$$P_M G_S P_M = P_M G_M P_M + P_M G_M g_M^{-1}(g_S - g_M) g_M^{-1} G_M P_M; \tag{2.1}$$

$$P_M G_S P_{\bar{M}} = P_M G_M g_M^{-1} g_S g_{\bar{M}}^{-1} G_{\bar{M}} P_{\bar{M}}; \tag{2.2}$$

$$g_S^{-1} = \frac{1}{s_A} {}'g_A^{(+)} g_A^{-1} - \frac{1}{s_B} {}'g_B^{(-)} g_B^{-1}, \tag{2.3}$$

where $P_M$ is the projector onto side M, for any G, $g$ is its surface projection, $g^{-1}$ is the inverse of $g$ *in the space of the matching surface*,

$${}'g^{(\pm)} = \lim_{z' \to z \pm 0} \frac{\partial G(z,z')}{\partial z} \tag{2.4}$$

and $s = {}'g^{(+)} - {}'g^{(-)}$ is the jump of the normal derivative, which is determined by the differential equation defining G. E.g., for a medium with effective mass $m$, this is $(-2m/\hbar^2)$ if the definition



$(E-H)G=\delta$ is used.

The question is: what is $G_M$? It is usually implied that $G_M$ is the GF of the infinite medium M. This would seem to restrict the usefulness of the analysis practically to the case of ideal interfaces, where M changes abruptly to M, so every $G_M$ can be obtained by standard procedures. However, nothing in the formal analysis requires this. $G_M$ can be the GF of any arbitrary *extended pseudomedium* (M) with the only condition that all extended pseudomedia must satisfy the same differential equation, namely that of the real Hamiltonian, on side M. To prove this consider the matching problem consisting of the actual M half on side M and anything else N on the other side. Let $G_{(M)}$ be the GF of this extended pseudomedium. Then

$$P_M G_{(M)} P_M = P_M G_M P_M + P_M G_M g_M^{-1}(g_{(M)} - g_M) g_M^{-1} G_M P_M; \tag{2.5}$$

whence, for M=A,

$${}'g_{(A)}^{(+)} = {}'g_A^{(+)} g_A^{-1} g_{(A)} \tag{2.6}$$

and, for M=B,

$${}'g_{(B)}^{(-)} = {}'g_B^{(-)} g_B^{-1} g_{(B)}. \tag{2.7}$$

Now match the extended pseudomedia (A) and (B). Then

$$g_{(s)}^{-1} = \frac{1}{s_A} {}'g_{(A)}^{(+)} g_{(A)}^{-1} - \frac{1}{s_B} {}'g_{(B)}^{(-)} g_{(B)}^{-1}. \tag{2.8}$$

It follows from (2.6) and (2.7) that

$$g^{-1}_{(s)} = g^{-1}_{s} \quad , \tag{2.9}$$

i.e., the secular matrix - yielding the secular equation $\det g_s^{-1}=0$ for the matching problem - is identically the same. Now consider the full GF for the pseudosystem. For $z,z'$ on the same side

$$P_M G_{(s)} P_M = P_M G_{(M)} P_M + P_M G_{(M)} g^{-1}_{(M)} (g_{(s)} - g_{(M)}) g^{-1}_{(M)} G_{(M)} P_M \quad . \tag{2.10}$$

Now, from (2.5):

$$P_M G_{(M)} g^{-1}_{(M)} = P_M G_M g^{-1}_M \quad ; \quad g^{-1}_{(M)} G_{(M)} P_M = g^{-1}_M G_M P_M \quad . \tag{2.11}$$

Use (2.5) for $P_M G_{(M)} P_M$ and (2.9) and (2.11) for the rest. Then

$$P_M G_{(s)} P_M = P_M G_s P_M \quad . \tag{2.12}$$

Likewise for the cross elements

$$P_M G_{(s)} P_{\tilde{M}} = P_M G_{(M)} g^{-1}_{(M)} g_{(s)} g^{-1}_{(\tilde{M})} G_{(\tilde{M})} P_{\tilde{M}} \tag{2.13}$$

and using (2.9) and (2.11),

$$P_M G_{(s)} P_{\tilde{M}} = P_M G_s P_{\tilde{M}} \quad , \tag{2.14}$$

i.e. the complete $G_{(s)}$ of the pseudosystem is equal to the actual $G_s$ of the actual system. The only limitation to this proof is seen in (2.6) and (2.7). The extended pseudomedium (A) *cannot* be chosen so that $'g_{(A)}(\cdot)$ vanishes, for then $g_{(A)}$ also vanishes and its inverse cannot be invoked in the subsequent proof. Physically this corresponds to the half medium A bounded by an infinite barrier, in which case obviously the pseudomedium (A) cannot be matched to any



other medium. Likewise $'g_{(B)}(\cdot)$ cannot vanish, for the same reason.

In conclusion: *Consider the real GF, $G_s$, of a Hamiltonian describing two media A, B matched at the interface. Then, whith the only limitation that $'g_{(A)}(\cdot)$ and $'g_{(B)}(\cdot)$ cannot vanish, the full SGFM analysis can be implemented, and the real $G_s$ can be found, by matching any arbitrary extended pseudomedia (M) provided each $G_{(M)}$ satisfies the real differential equation on side M.*

The freedom to choose any $G_{(M)}$ with arbitrary boundary condition at the interface can be used in practice either to define a $G_{(M)}$ which can be more easily evaluated or else to simplify the calculation. An example will be seen presently.

Now consider the two interface problem A-*l*-B-*r*-C, where A,B,C are the media matched, in this order, at the left *l* and right *r* surfaces. This corresponds to various situations of physical interest, such as a quantum well (A=C,B a well), a layer B on a substrate C (A=vacuum), or a barrier B between A and C. Consider the GF $G_{AB}$ which describes media A and B matched at *l*. The result of matching $G_{AB}$ with $G_C$ at *r* is $G_{ABC}$, the complete - real - GF, Gs, of the composite system A-*l*-B-*r*-C. Now, $G_{AB}$ can be replaced by any permitted pseudo $G_{(AB)}$ which satisfies the real differential equation from $-\infty$ to *r*, and this can then be matched to $G_C$, or to any permitted pseudo $G_{(C)}$ which satisfies the real differential equation from *r* to $\infty$. It follows that the three media can be arbitrary pseudised, each one satisfying the real differential equation in its own domain, i.e. the full SGFM analysis can be implemented, and the correct $G_s$ can be found, by replacing $G_A$, $G_B$,

$G_e$ by arbitrary pseudo GF's $G_{(A)}$, $G_{(B)}$, $G_{(C)}$ provided, (i) every $G_{(\alpha)}$ satisfies the real differential equation in domain M - finite or infinite - and, (ii)

$$'g^{(+)}_{(A)l} \neq 0, \quad 'g^{(-)}_{(B)l} \neq 0, \quad 'g^{(+)}_{(B)r} \neq 0, \quad 'g^{(-)}_{(C)r} \neq 0 \ . \tag{2.15}$$

The general A,B,C sandwich can be studied by defining the matching surface to consist of $l$ and $r$, so the surface projections become 2×2 supermatrices (Velasco and García-Moliner, 1979). The matching formula is then

$$\check{G}_s^{-1} = \check{s}_e^{-1}\ '\tilde{G}_e\tilde{G}_e^{-1} - \tilde{s}_B^{-1}\ '\tilde{G}_B\tilde{G}_B^{-1} \ , \tag{2.16}$$

where

$$\check{s}_e^{-1} = \begin{Vmatrix} s_A^{-1} & 0 \\ 0 & s_C^{-1} \end{Vmatrix} \ ; \ '\tilde{G}_e = \begin{Vmatrix} 'g^{(+)}_{Al} & 0 \\ 0 & 'g^{(-)}_{Cr} \end{Vmatrix} \ ; \ \tilde{G}_e = \begin{Vmatrix} g_{Al} & 0 \\ 0 & g_{Cr} \end{Vmatrix} \tag{2.17}$$

while

$$'\tilde{G}_B = \begin{Vmatrix} 'g^{(-)}_{Bl} & 'g^{(+)}_{Bl}g^{-1}_{Bl}G_{B,lr} \\ -'g^{(-)}_{Br}g^{-1}_{Br}G_{B,rl} & -'g^{(+)}_{Br} \end{Vmatrix} \ ; \tilde{G}_B = \begin{Vmatrix} g_{Bl} & G_{B,lr} \\ G_{B,rl} & g_{Br} \end{Vmatrix} . \tag{2.18}$$

The choice of a pseudo $G_{(\alpha)}$ such that

$$'g^{(+)}_{(B)l} = 0 = 'g^{(-)}_{(B)r} \tag{2.19}$$



is permitted. If such a $G_{(\alpha)}$ can be found then $s_\alpha^{-1}\ '\check{G}_\alpha$ becomes simply the negative of the unit matrix, with considerable simplification in the evaluation of the secular matrix (2.16).

The case of the superlattice is similarly studied (García-Moliner and Velasco, 1986). The two constituent media - C=A in this case - can also be pseudised so that each $G_{(\alpha)}$ satisfies the real differential equation in its own finite slab and the corresponding forbidden boundary conditions are avoided.

The usefulness of this formal analysis depends in practice on being able to find the desired $G_\alpha$'s for a given Hamiltonian. This question will be studied presently.

## 3. Transfer matrix versus Green function.

Consider a given onedimensional differential equation. Let $\Psi$, $\Psi'$ be one eigenfunction and its derivative. The transfer matrix $M(z,z')$, which transfer *from* $z'$ *to* $z$, is defined by

$$\begin{pmatrix} \Psi \\ \Psi' \end{pmatrix}_z = \begin{Vmatrix} M_{11}(z,z') & M_{12}(z,z') \\ M_{21}(z,z') & M_{22}(z,z') \end{Vmatrix} \cdot \begin{pmatrix} \Psi \\ \Psi' \end{pmatrix}_{z'} \ . \tag{3.1}$$

The general mathematical properties of the transfer matrix (TM) and its physical applications in the case of the Schrödinger equation have been discussed elsewhere (Mora et al., 1985).

For a onedimensional Schrödinger equation with a constant potential V,

$$M(z,z') = \begin{Vmatrix} \cos\phi & K^{-1}\sin\phi \\ -K\sin\phi & \cos\phi \end{Vmatrix} ; \quad \phi = K(z-z') \quad , \tag{3.2}$$

where, in terms of E, the kinetic energy of motion in the z direction,

$$K = \begin{cases} [(E-V)2m/\hbar^2]^{1/2} \quad , \quad E>V \ ; \\ i[(V-E)2m/\hbar^2]^{1/2} = i\Omega \quad , \quad E<V \ . \end{cases} \tag{3.3}$$

Any given potential V(z) can be approximated to any desired accuracy in the (z',z), internal by taking a succession of N steps from $z'=z_0$ to $z_1$, to $z_2$,...to $z_{N-1}$, to $z=z_N$, with $V=V_n=$const. for every $n$-th interval from $z_{n-1}$ to $z_n$. Within each interval (3.2) can be used with the local value of $V_n$. The transfer matrix M(z,z') can then be obtained to any desired accuracy by using the multiplicative property

$$M(z,z') = M(z,z_{N-1})M(z_{N-1},z_{N-2})\ldots M(z_2,z_1)M(z_1,z') \ . \tag{3.4}$$

This provides a very simple and efficient algorithm in practice. It is therefore interesting to relate the GF of a differential equation to its TM.

Now, given any two linearly independent solutions $g_1(z)$, $g_2(z)$ we can write



$$G(z,z') = \begin{cases} [A\,g_1(z')+B\,g_2(z')][C\,g_1(z)+D\,g_2(z)] & z\leq z' \\ [C\,g_1(z')+D\,g_2(z')][A\,g_1(z)+B\,g_2(z)] & z\geq z' \ . \end{cases} \tag{3.5}$$

This ensures the conditions

$$G(z,z-0) = G(z,z+0) \ ; \ G(z,z') = G(z',z) \ . \tag{3.6}$$

Furthermore, the condition

$$AD-BC = s/w \ , \ w = g_1g_2' - g_2g_1' \tag{3.7}$$

ensures that '$g$'' has the correct jump s. A change of basis

$$g_1(z) = a_{11}f_1(z) + a_{12}f_2(z); \ g_2(z) = a_{21}f_1(z) + a_{22}f_2(z) \tag{3.8}$$

leads to the same form (3.5) with $g_1, g_2$ replaced by $f_1, f_2$ and A,B,C,D replaced by A',B',C',D' with

$$\begin{aligned} A' &= a_{11}A + a_{21}B \ , \\ B' &= a_{12}A + a_{22}B \ , \\ C' &= a_{11}C + a_{21}D \ , \\ D' &= a_{12}C + a_{22}D \ . \end{aligned} \tag{3.9}$$

It is easily seen that the jump condition (3.7) is then

$$A'D'-B'C' = s/w', \ w' = f_1f_2' - f_2f_1' \ , \tag{3.10}$$

with the wronskian w' of the new basis $f_1, f_2$. Now define $f_1, f_2$ to form a canonical basis at a fixed point $z_0$:

$$f_1(z) = h_1^{z_0}(z): \qquad f_1(z_0) = 1 \ , \ [\frac{df_1(z)}{dz}]_{z_0} = 0 \ ;$$

$$f_2(z) = h_2^{z_0}(z): \qquad f_2(z_0) = 0 \ , \ [\frac{df_2(z)}{dz}]_{z_0} = 1 \ ; \tag{3.11}$$

so w'=1. Now, from (3.1), for $\Psi = f_1, f_2$:

$$f_1(z) = M_{11}(z,z_0) \ ; \ f_2(z) = M_{12}(z,z_0) \ . \tag{3.12}$$

The new Wronskian w' is simply equal to unity. Putting $\alpha$ , $\beta$, $\gamma$, $\delta$ for the values of A',B',C',D' corresponding to this case it follows that

$$G(z,z') = \begin{cases} [\alpha M_{11}(z',z_0)+\beta M_{12}(z',z_0)][\gamma M_{11}(z,z_0)+\delta M_{12}(z,z_0)], & z \leq z' ; \\ [\gamma M_{11}(z',z_0)+\delta M_{12}(z',z_0)][\alpha M_{11}(z,z_0)+\beta M_{12}(z,z_0)], & z \geq z' \end{cases} \tag{3.13}$$

with

$$\alpha\delta - \beta\gamma = s \ . \tag{3.14}$$

The derivative with respect to the first argument, z, is then (Mora et al., 1985)



$$'G(z,z') = \begin{cases} [\alpha M_{11}(z',z_0)+\beta M_{12}(z',z_0)][\gamma M_{21}(z,z_0)+\delta M_{22}(z,z_0)], & z \leq z' ; \\ [\gamma M_{11}(z',z_0)+\delta M_{12}(z',z_0)][\alpha M_{21}(z,z_0)+\beta M_{22}(z,z_0)], & z \geq z' \end{cases} \tag{3.15}$$

Thus the GF can be known if the TM is known and this, as has just been explained, can be done with great numerical ease for any potential of arbitrary shape between z' and z.

## 4. Surface Green Function Matching for a sandwich ABC with arbitrary potential in B.

Now consider again the general ABC sandwich of Section 2. Suppose $G_A$ and $G_C$ can be evaluated, but B has a potential given in numerical form and the construction of $G_B$ by standard methods becomes practically intractable. The information embodied in the TM for B, which is easily evaluated numerically, can then be used to obtain those elements of $G_B$ entering the matching formula (2.18). Indeed, taking $z_0$ at $l$ and then $z$ and/or $z'$ at either $l$ or $r$ and defining

$$m_{ij} = M_{ij}(r,l) \tag{4.1}$$

for the TM which transfers across the potential $V_B$, (3.9) and (3.10) yield

$$g_l = \alpha\gamma \ ; \ G_{lr} = G_{rl} = \gamma(\alpha m_{11}+\beta m_{12}); \ g_r = (\alpha m_{11}+\beta m_{12})(\gamma m_{11}+\delta m_{12});$$

$$'g_l^{(+)} = \alpha\delta \ ; \ 'g_l^{(-)} = \beta\gamma; \ 'g_r^{(+)} = (\alpha m_{11}+\beta m_{12})(\gamma m_{21}+\delta m_{22});$$

$$'\varphi_r^{(-)} = (\gamma m_{11}+\delta m_{12})(\alpha m_{21}+\beta m_{22}) \quad . \tag{4.2}$$

The jump condition at $l$ is immediately obvious and it is easily checked at $r$ by using the general property (Mora et al.,1985) det m=1.

Using (4.2) in (2.16) through (2.18) yields

$$\tilde{G}_s^{-1} = \begin{Vmatrix} \frac{1}{s_A}\,'\varphi_{Al}^{(+)}\varphi_{Al}^{-1}+\frac{1}{s_B}\left(\frac{m_{11}}{m_{12}}\right)_B & -\frac{1}{m_B}\left(\frac{1}{m_{12}}\right)_B \\ -\frac{1}{m_B}\left(\frac{1}{m_{12}}\right)_B & -\frac{1}{s_C}\,'\varphi_{Cr}^{(-)}\varphi_{Cr}^{-1}+\frac{1}{m_B}\left(\frac{m_{22}}{m_{12}}\right)_B \end{Vmatrix} \tag{4.3}$$

where $m_B$ is the mass in medium B.

Now, the concept ot the TM makes no reference to the boundary conditions. The freedom in the choice of parameters left in (3.13) shows that for a given M there are different G's, corresponding to different boundary conditions. According to the theorem proved in Section 2 all these are different pseudo G's which yield uniquely the same final result for the matching problem. This is reflected, indeed, in the fact that by starting from (4.2), which contains arbitrary and undefined parameters, one obtains (4.3) from which all parameters, have disappeared, except for the combination $(\alpha\delta-\beta\gamma)$ in the denominators of the B terms which, by (3.14), is precisely the jump $s_B$. Thus the final result contains all the information about B: the $m_{ij}$'s give the form and $s_B$ gives the amplitude. The matching problem has been solved without knowing $G_B$.

As shown in the SGFM analysis (García-Moliner and



Velasco, 1986) from the secular matrix one obtains the results of physical interest for a given situation. For example for the quantum well problem the secular equation for the bound states is

$$\det|G_s^{-1}| = 0 \quad , \tag{4.4}$$

where one needs only use (4.3). This yields

$$\frac{m_B}{m_C}\,'\varphi_{Cr}^{(-)}\varphi_{Cr}^{-1}\,m_{11} - \frac{m_B}{m_A}\,'\varphi_{Al}^{(+)}\varphi_{Al}^{-1}\,m_{22} - m_{21} +$$

$$\frac{m_B}{m_A}\frac{m_B}{m_C}\,'\varphi_{Al}^{(+)}\varphi_{Al}^{-1}\,'\varphi_{Cr}^{(-)}\varphi_{Cr}^{-1}\,m_{12} = 0 \tag{4.5}$$

valid for any $G_A$ and $G_C$. In particular, if $V_A$ and $V_C$ are constant this yields the result known from TM analysis for this case (Pérez-Alvarez and Rodriguez-Coppola, 1987).

When B is a barrier the interest centres on the reflection or transmission probabilities. For incidence from side A the corresponding amplitudes are

$$f_R = (\tilde{G}_{s,11}-\varphi_{Al})\varphi_{Al}^{-1} \tag{4.6}$$

for the reflection amplitude and

$$f_T = \tilde{G}_{s,rl}\varphi_{Al}^{-1} \tag{4.7}$$

for the wavefunction transmission amplitude. The information on the matching process is contained in the secular matrix (4.3), of which the $\tilde{G}_s$ entering (4.6) and (4.7) is the inverse. Thus this

information is also embodied in $f_R$ and $f_T$. In particular, for $V_A$ and $V_C$ constant the transmission probability is

$$T = |f_T|^2 \frac{K_C/m_C}{K_A/m_A} \quad . \tag{4.8}$$

Using (4.3) this yields

$$T = \frac{4\, K_C K_A (m_C/m_A)}{[K_C m_{11} + K_A m_{22}(m_C/m_A)]^2 + [K_A K_C m_{12}(m_B/m_A) - m_{21}(m_C/m_B)]^2} \quad , \tag{4.9}$$

again in agreement with the result known from TM analysis for this case (Pérez-Alvarez and Rodriguez-Coppola, 1987).

The connection between the TM and SGFM formalisms has thus been established and illustrated with some obtainable analytical formulae. The key result is in (4.3) and its practical interest lies in the fact that it can be readily used for a numerical calculation. This will be demonstrated in the next Section.

## 5. Application. Bound states of a parabolic quantum well.

Pötz and Ferry (1985) have calculated the bound states of a 507 Å thick parabolic quantum well generated by layers of GaAs and $Ga_{(1-x)}Al_xAs$. The quantised levels for zero momentum parallel to the interfaces ($\kappa$=0) were calculated for an (eight-band) envelope function model including remote-band effects in second order perturbation theory. The numerical solution of the Schrödinger equation for this problem entails a very substantial



amount of computation. These results will be taken here as a reference term to compare with.

Now for $\kappa$=0 in the envelope function models one expects the different bands to decouple for zincblende structure (Altarelli, 1985). The present calculation was then carried out in the following manner: The same input parameters as those of Pötz and Ferry (1985) were used and the different bands were treated separately. The matching problem for each one was solved by using (4.3) and the corresponding quantised bound state levels obtained from (4.4). The transfer matrix across the parabolic quantum well was evaluated by subdividing it in *forty* steps and the calculation done on a personal computer. The results are shown in Table I and compared with those of Pötz and Ferry (1985). The agreement is seen to be excellent.

Table I

On an Olivetti personal computer one of the eigenvalues is obtained in little more than two minutes. The entire calculation required for the twelve eigenvalues given in Table I takes about half an hour. Some checks were performed on the accuracy of the forty step approximation. To obtain an eigenvalue by subdividing in 100 steps takes five minutes; if 200 steps are used then it takes ten minutes. In all checks performed no significant changes were found within tenths of a meV. This demonstrates the practical usefulness of the connection found in Sections 3 and 4 between the TM in the sense of Mora et al. (1985) and GF and, in particular, the practical usefulness of the secular equation obtained from (4.3).

## 6. Conclusions

The limitation of the SGFM analysis in practice is that there may be cases in which there is no easy way to evaluate the GF of one of the constituent media. For ABC configurations this often arises when B is 'difficult' in this sense. The TM of Mora et al (1985) provides an algorithm with which the Schrödinger equation in any arbitrary potential can be solved with great numerical ease. The combination of these two concepts provides a hybrid approach in which the information obtained from the TM is inserted in its precise place within the SGFM analysis, so in the end one can in practice match $G_A$, $G_B$ and $G_C$ without really knowing $G_B$. This yields a very practical secular equation, as demonstrated by the application presented in Section 5.

There are some obvious extensions of the analysis presented in this paper. One is to exploit fully the possibility of designing arbitrary pseudo GF's as proved in Section 2. This need not require invoking the TM but is an interesting possibility in itself. As an example, the SGFM matching equation for a finite square quantum well in an external electric field has been obtained in analytical form (Glasser and Garcia-Moliner, 1987) by using for the B region the field dependent GF which consists of a product of the linear combinations $(A_i - iB_i)$ and $(B_i - iA_i)$ of the Airy functions. In the zero field limit this yields the actual GF for electrons in a constant potential. However, it follows from Section 2 that one can equally use a pseudo GF consisting simply of the products of $A_i$ and $B_i$ alone. In the zero field limit this yields not the real GF but a pseudo GF which satisfies the same differential equation, but the algebra needed to obtain the secular



equation for finite field is substantially simpler and, of course, yields exactly the same result.

Another way to simplify the calculation for an ABC sandwhich is to form the pseudo $G_{(B)}$ according to (2.19). This can be very useful in the study of vector fields -e.g. elastic or piezoelectric media - when the GF's involved are 3×3 or 4×4 matrices. The way to design such a pseudo GF is to use the scheme of (3.5), where the independent solutions can be written down analytically - e.g. the three independent plane wave solutions with the three elastic wave velocities running in either direction. Again, this need not yet introduce the concept of TM, although it can be combined with the TM, if desired, by using (3.8).

Now, the hybrid approach demonstrated by the practical application of Section 5 has also immediate extensions. One is to the full threedimensional case. By Fourier transforming in two dimensions the resulting problem is onedimensional, but for given twodimensional wavevector $\kappa$ the crystal potential mixes all relevant components where $\kappa'-\kappa$ is a reciprocal wavevector of the twodimensional Brillouin zone. The wavefunction then is a vector, the GF a matrix and the TM a 2×2 supermatrix.

The mathematical basis required for this problem is given in the work of Mora et al. (1985) and so the way to effect the extension to the full threedimensional case is clear in principle. The other obvious extension of the hybrid method is to include selfconsistency into it, the way to do it being to obtain the charge density from the local density of states, which in turn is obtainable from the imaginary part of the $G_B$ matched for each cycle of the selfconsistent calculation.

Work on these problems is currently in progress.

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Table I

| | Lowest conduction | | Heavy holes | | Light holes | |
|---|---|---|---|---|---|---|
| | (A) | (B) | (A) | (B) | (A) | (B) |
| $E_1$ | 1531.1 | 1531.1 | -4.5 | -4.5 | -10.1 | -10.1 |
| $E_2$ | 1555.0 | 1554.8 | -13.4 | -13.4 | -30.4 | -30.4 |
| $E_3$ | 1578.8 | 1578.6 | -22.3 | -22.4 | -49.6 | -50.6 |
| $E_4$ | 1601.9 | 1602.3 | -31.2 | -31.3 | -68.9 | -70.8 |

Table I.- Quantised subband levels in meV for the parabolic quantum well described in the text. (A): Pötz and Ferry. (B): Present calculation.