Continuity conditions for the wave function of a particle with a position-dependent mass in a laser field

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The continuity conditions for the wave function of a particle with a position-dependent mass and interacting with an oscillating field are derived. One-dimensional motion is assumed and the potential is represented as a series of constant steps. The method introduces discontinuities in the potential and the mass and the matching conditions need to be reformulated to take into account the presence of the field. An application is made to the calculation of the transmissivity of an electron with a sector-dependent effective mass in a nanostructure. The use in each sector of the wave equation without the A^2 term is necessary to ensure convergence with respect to the number of channels.

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I. INTRODUCTION

The matching conditions to be fulfilled by the wave function at a potential discontinuity are discussed in all quantum mechanics textbooks (see, for example, [1,2]). For one-dimensional motion, the conditions are very simple: the wave function and its derivative with respect to the coordinate have to be continuous. This is the basis for the solution of elementary bound and scattering-state problems such as the square well, the potential step or tunneling through a barrier. An extension is needed for the treatment of resonant tunneling through a double-barrier nanostructure when the variation with composition of the effective electron mass is taken into account [3]: the ratio derivative of the wave function over mass has to be continuous in order to ensure continuity of the current. We have in view a further extension: the particle is assumed to interact with an oscillating field. The Hamiltonian is now time dependent. This is the case if a laser is used to modify the transmissivity, with the laser field being represented classically. Although a very simple modification of the matching conditions used in the field-free case with variable mass is needed, it does not appear that the literature mentions it, not to speak of its implementation in effective calculations. Section II derives the new matching conditions, with a minimum number of assumptions about the problem at hand. One-dimensional motion is assumed and the potential is represented as a series of steps, with a mass that may change with the step. We give in Sec. III, the form of the functions to be used in each step (called also a sector). Some applications are given in Sec. IV to demonstrate the validity of the proposed relations.

II. MATCHING AT A DISCONTINUITY AND CONTINUITY OF CURRENT

A discontinuity in the present context concerns both the potential and the mass. We consider a solution of a wave equation with a time-dependent Hamiltonian and we look for the conditions to be satisfied at the discontinuity. We have to ensure two types of continuity to match the wave functions on both sides of the discontinuity:

(1) Continuity of the wave function $\Psi(x,t)$ in space and time.

(2) Continuity in space and time of some function of its derivative to ensure continuity of current.

Continuity of the wave function in space is easily satisfied by writing, if X_j is the point that is common to sectors j and $j+1$,

$$\Psi_j(x,t)|_{x=X_j}=\Psi_{j+1}(x,t)|_{x=X_j}. \tag{1}$$

Before discussing how to impose continuity in time, we discuss the matching conditions involving the derivative of the wave function with respect to space. Continuity in time will be done in the same way for the two categories of conditions. The derivation follows, with appropriate changes, that made for a position-dependent mass $m(x)$ in the field-free case [3]. We start from the wave equation, integrate across the discontinuity X_j of the potential between sectors j and $j+1$ and perform a limiting procedure

$$\lim_{\epsilon\to 0}\int_{X_j-\epsilon}^{X_j+\epsilon}\left[H-E-i\frac{\partial}{\partial t}\right]\Psi(x,t)dx=0. \tag{2}$$

This relation is a direct consequence of the time-dependent wave equation. In the case where the field $f(t)$ is a periodic function of time, we can look at it as an equation satisfied by the Floquet eigenfunction. The Hamiltonian can be derived from that of the field-free case [4]

$$H^0=\frac{1}{2}p_x\frac{1}{m(x)}p_x+V(x), \tag{3}$$

by the substitution $p_x\rightarrow p_x-f(t)$, thus producing

$$H=\frac{1}{2}[p_x-f(t)]\frac{1}{m(x)}[p_x-f(t)]+V(x). \tag{4}$$

Let us explicit the kinetic term

$$T=[p_x-f(t)]\frac{1}{2m(x)}[p_x-f(t)]=\frac{1}{2}p_x\frac{1}{m(x)}p_x$$
$$-\frac{f(t)}{2}\left[p_x\frac{1}{m(x)}+\frac{1}{m(x)}p_x\right]+\frac{f^2(t)}{2m(x)}. \quad (5)$$

The function $m(x)$ has a discontinuity at $x=X_j$. All the integrals present in Eq. (2) involve bounded functions except those containing the derivative of $1/m(x)$. The former type of integrals go, therefore, to zero as $\epsilon\rightarrow 0$. To examine the nature of the singularity present in the latter class, we write close to the discontinuity

$$\frac{1}{m(x)}=\left(\frac{1}{m^R}-\frac{1}{m^L}\right)\theta(x-X_j)+\frac{1}{m^L}, \quad (6)$$

$\theta(x-X_j)$ being the Heaviside function, 0 for $x<X_j$ and 1 for $x>X_j$. m^R and m^L are the masses on the right and on the left of the discontinuity. We have for the derivative of $1/m(x)$,

$$\frac{d}{dx}\frac{1}{m(x)}=\left(\frac{1}{m^R}-\frac{1}{m^L}\right)\delta(x-X_j). \quad (7)$$

Retaining only the terms depending on this derivative, we are left with

$$\lim_{\epsilon\rightarrow 0}\int_{X_j-\epsilon}^{X_j+\epsilon}\left[-\frac{1}{2}\frac{\partial}{\partial x}\frac{1}{m(x)}\frac{\partial\Psi(x,t)}{\partial x}+i\frac{f(t)}{2}\frac{\partial}{\partial x}\frac{1}{m(x)}\Psi(x,t)\right]dx=0. \quad (8)$$

Equation (7) is in fact not needed, because the integrals contain only derivatives of functions with respect to x. The integration is straightforward and produces

$$-\frac{\Psi'^R}{2m^R}+\frac{\Psi'^L}{2m^L}+i\frac{f(t)}{2}\left(\frac{\Psi^R}{2m^R}-\frac{\Psi^L}{2m^L}\right). \quad (9)$$

Another instructive way to write this relation is

$$\frac{1}{m^R}[p_x-f(t)]\Psi^R(x,t)|_{x=X_j}=\frac{1}{m^L}[p_x-f(t)]\Psi^L(x,t)|_{x=X_j}. \quad (10)$$

This is the matching relation involving the derivative of the wave function with respect to position. It is obtained from that of the field-free case by the same substitution as used to derive the Hamiltonian.

We now investigate the condition for continuity of current. We start from the time-dependent wave equation written

$$\left[-i\frac{\partial}{\partial x}-f(t)\right]\frac{1}{2m(x)}\left[-i\frac{\partial}{\partial x}-f(t)\right]\Psi(x,t)=i\frac{\partial\Psi(x,t)}{\partial t}. \quad (11)$$

Multiplication of this equation by $\Psi^*(x,t)$, of its complex conjugate by $\Psi(x,t)$ and subtracting the second equation from the first produces the conservation relation

$$\frac{\partial\Psi^*(x,t)\Psi(x,t)}{\partial t}+\frac{\partial J_x}{\partial x}=0, \quad (12)$$

with, after some rearrangement

$$\frac{\partial J_x}{\partial x}=\frac{1}{2i}\frac{\partial}{\partial x}\left[\Psi^*(x,t)\frac{1}{m(x)}\frac{\partial\Psi(x,t)}{\partial x}-\Psi(x,t)\frac{1}{m(x)}\frac{\partial\Psi^*(x,t)}{\partial x}\right]-f(t)\frac{\partial}{\partial x}\left[\frac{\Psi^*(x,t)\Psi(x,t)}{m(x)}\right]. \quad (13)$$

Integration of this relation provides us with

$$J_x=\frac{1}{2i}\left[\Psi^*(x,t)\frac{1}{m(x)}\frac{\partial\Psi(x,t)}{\partial x}-\Psi(x,t)\frac{1}{m(x)}\frac{\partial\Psi^*(x,t)}{\partial x}\right]-f(t)\left[\frac{\Psi^*(x,t)\Psi(x,t)}{m(x)}\right]. \quad (14)$$

If $m(x)=m$ and $f(t)=0$ the usual current is recovered

$$J_x=\frac{1}{2mi}\left[\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}-\Psi(x,t)\frac{\partial\Psi^*(x,t)}{\partial x}\right]. \quad (15)$$

If $m(x)=m$ and $f(t)\neq 0$ the current has an additional term

$$J_x=\frac{1}{2mi}\left[\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}-\Psi(x,t)\frac{\partial\Psi^*(x,t)}{\partial x}\right]-\frac{f(t)}{2m}\Psi^*(x,t)\Psi(x,t). \quad (16)$$

This is the current in the presence of an electromagnetic field discussed in the literature [2,5], $f(t)$ being in that case the vector potential.

Continuity of current requires that

$$J_x(X_j-\epsilon)=J_x(X_j+\epsilon). \quad (17)$$

This condition gives immediately

$$\Psi^{R*}[(1/i)\Psi^{R'}-f(t)\Psi^R](1/m^R)-\Psi^R[(1/i)\Psi^{R'*}+f(t)\Psi^{R*}]1/m^R$$
$$=\Psi^{L*}[(1/i)\Psi^{L'}-f(t)\Psi^L](1/m^L)-\Psi^L[(1/i)\Psi^{L'*}+f(t)\Psi^{L*}]1/m^L, \quad (18)$$

or also

$$(\Psi^{R*}/m^R)[p_x-f(t)]\psi^R-(\Psi^R/m^R)[p_x+f(t)]\Psi^{R*}$$
$$=(\Psi^{L*}/m^L)[p_x-f(t)]\psi^L-(\Psi^L/m^L)[p_x+f(t)]\Psi^{L*}. \quad (19)$$

We can now observe that using the matching condition [Eq. (10)] and its complex conjugate we prove the continuity of current. However, from the condition for continuity of current alone, because of its complex nature, we are not able to derive the matching conditions.

Continuity in time could be imposed by identification of the Fourier expansions of the functions present in the two types of space matching [Eqs. (1) and (10) [6–9]]. It has been shown previously [10] that a simple and efficient procedure consists in equaling the functions at a set of times distributed uniformly along a period of the field.

III. SECTOR GORDON-VOLKOV WAVE FUNCTIONS

The previous matching conditions will now be applied in the context of the calculation of the transmissivity of a particle interacting with an oscillating field. The method we follow goes back to Sacks and Szöke [6] and Kaminski [7] who developed a formalism to treat the scattering of a particle incident on a stepwise constant potential. The oscillating field can be of arbitrary intensity. Kaminski has shown [7], through the use of transfer matrices [1,11,12] how to treat a potential of arbitrary shape, considered as the limit, as the number of steps is increased, of a stepwise constant potential. In each step, the wave function is written as a linear combination of Gordon-Volkov (GV) waves for a constant potential. The number of such waves depends on the number of quanta that can be effectively exchanged between the particle and the field. We have described elsewhere [13] our own implementation of the transfer-matrix procedure. The method was applied to resonant tunneling through a biased double barrier by ''slicing'' the potential into a series of steps. The mass was assumed to be the same everywhere.

A sector is a region of constant potential. In each sector the time-dependent wave function is a linear combination of solutions of the wave equation with a time-dependent term $f(t)$ in the Hamiltonian. For an electromagnetic field in the long wavelength approximation $f(t)$ is the vector potential $A(t)$. Let j be the index of a sector. The wave equation in velocity gauge is, in sector j, in atomic units

$$i\frac{\partial\psi_j(x,t)}{\partial t}=\left[\frac{1}{2m_j}\left(\frac{1}{i}\frac{\partial}{\partial x}-f(t)\right)^2+V_j\right]\psi_j(x,t), \tag{20}$$

where V_j and m_j are the values assumed by the potential and the mass in this region. A solution with unit flux normalization is

$$\psi^{\pm}_{j,n}(x,t)=\sqrt{\frac{m_j}{k_{j,n}}}\exp[-iE_nt]\exp\left[-\frac{i}{2m_j}\int^t f^2(t')dt'\right]\times\exp\left[\pm ik_{j,n}(x+m_j^{-1})\int^t f(t')dt'\right]. \tag{21}$$

The energy is $E_n=E+n\omega$, where E is the incident energy. This means that we have allowed for an exchange of n quanta, n being either positive (absorption) or negative (emission). We have for the wave numbers the relation $k^2_{j,n}=2m_j[E_n-V_j]$. If $f(t)=A_0\cos(\omega t)$, the explicit form of this function is

$$\psi^{\pm}_{j,n}(x,t)=\sqrt{\frac{m_j}{k_{j,n}}}\exp[-iE_nt]\exp\left[-\frac{iA_0^2t}{4m_j}\right]\times\exp\left[-i\frac{A_0^2\sin(2\omega t)}{8m_j\omega}\right]\times\exp\left[\pm ik_{j,n}\left(x+\frac{A_0\sin(\omega t)}{m_j\omega}\right)\right]. \tag{22}$$

The normalization is easily checked through the fact that it is determined only by the x-dependent factor, which is the same as that of a free wave of a free electron, $\sqrt{m_0/k}\exp[\pm ikx]$.

We also note, for further discussion, that a unitary transformation can eliminate the $f^2(t)$ term from the wave equation. The new wave function is

$$\tilde{\psi}^{\pm}_{j,n}(x,t)=\exp\left[-\frac{i}{2m_j}\int^t f^2(t')dt'\right]\psi^{\pm}_{j,n}(x,t). \tag{23}$$

The solution takes the simple form

$$\tilde{\psi}^{\pm}_{j,n}(x,t)=\sqrt{\frac{m_j}{k_{j,n}}}\exp[-iE_nt]\times\exp\left[\pm ik_{j,n}\left(x+\frac{A_0\sin(\omega t)}{m_j\omega}\right)\right]. \tag{24}$$

When referring to such sector functions we will speak of the reduced velocity gauge to emphasize that the $f^2(t)$ [or $A^2(t)$] term has been eliminated from the wave equation that now reads

$$i\frac{\partial\tilde{\psi}_j(x,t)}{\partial t}=\left[-\frac{1}{2m_j}\frac{\partial^2}{\partial x^2}+\frac{i}{m_j}f(t)\frac{\partial}{\partial x}+V_j\right]\tilde{\psi}_j(x,t), \tag{25}$$

The discussion of the matching condition to be given in the previous section does not depend on the choice of gauge. It would appear that the velocity gauge is to be preferred to the reduced velocity gauge, since the unitary transformation between the two gauges is mass-dependent and, therefore, sector dependent: however, the numerical studies to be presented in Sec. IV point to a definitive superiority of reduced velocity gauge.

We can give now the general solution to be used in sector j. This is, in velocity gauge

$$\Psi_j(x,t)=\sum_{n=-N}^{n=+N}[t_n^j\psi^+_{j,n}(x,t)+r_n^j\psi^-_{j,n}(x,t)]. \tag{26}$$

In reduced velocity gauge, the sector functions of Eq. (22) are to be replaced by those of Eq. (24). N is the maximum of quanta that can be exchanged between particle and field. For simplicity we assume equality of the maximum numbers of either absorbed or emitted photons. Continuity in time of the wave function and of its derivative should provide each half the number of the relations needed to obtain a square matrix. The times are $\tau_i=[2\pi(i-1)]/(2N+1)\omega$, with i

$=1,2,\ldots,2N+1$. There are $2(2N+1)$ amplitudes in the wave functions on both sides of a discontinuity.

The amplitudes of the GV waves on the left and on the right of the discontinuity can be arranged as two column vectors

$$\mathbf{a}^{\mathbf{L}}=\begin{pmatrix}\mathbf{t}^{L}\\ \mathbf{r}^{L}\end{pmatrix}, \quad \mathbf{a}^{\mathbf{R}}=\begin{pmatrix}\mathbf{t}^{R}\\ \mathbf{r}^{R}\end{pmatrix}, \tag{27}$$

where $\mathbf{t}$ and $\mathbf{r}$ are column vectors made of all transmission and reflection amplitudes present in the function given in Eq. (26). The matching conditions at discontinuity X_j can be arranged in matrix form

$$\mathbf{M}^{R}(X_j)\mathbf{a}^{\mathbf{R}}=\mathbf{M}^{L}(X_j)\mathbf{a}^{\mathbf{L}}. \tag{28}$$

Once the propagation from left to right has been achieved, whatever method is being used, the result relating the amplitudes in the left and right asymptotic regions can be given the compact form

$$\mathbf{a}^{\mathrm{Right}}=\mathcal{M}\mathbf{a}^{\mathrm{Left}}. \tag{29}$$

$\mathcal{M}$ is the global transfer matrix obtained from the sequence of matching operations. The usual boundary conditions can be introduced at this stage: unit amplitude in the incoming channel with zero photon ($t_0^{\mathrm{Left}}=1$) and no reflected waves in the right region ($r_n^{\mathrm{Right}}=0$). This determines all r_n^{Left} and all t_n^{Right}. Assuming that in the left and right asymptotic regions the potentials are constant (but not necessarily identical), the reflection and transmission probabilities are given in terms of the r_n's in the region of the incident wave and of the t_n's in the region of the transmitted waves as

$$R_n=|r_n^{\mathrm{Left}}|^2, \quad T_n=|t_n^{\mathrm{Right}}|^2. \tag{30}$$

This simple form is due to our choice of normalization.

IV. TRANSMISSIVITY THROUGH A NANOSTRUCTURE

The study of the transmissivity of a particle through a system of barriers and wells is of great importance for the understanding of many semiconductors devices [14]. The variation of the potential is obtained by using semiconductors of various structures. For instance, for a $\mathrm{Al}_{\chi}\mathrm{Ga}_{1-\chi}\mathrm{As}$ material, according to Adachi [15], the potential is

$$V=0.6(1.15\chi+0.37\chi^2), \tag{31}$$

in eV. The corresponding effective mass is

$$m(\chi)=0.067+0.083\chi, \tag{32}$$

in units of the free electron mass m_0. The sectors introduced previously can be associated to physically distinct potential regions, with eventually different effective masses. For a complicated potential the sectors represent an approximation to the true potential, to be tested later by increasing the number of sectors until there is convergence of the transition probabilities An example of the first case is a double-barrier device without a bias voltage and with barriers made of $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.5}\mathrm{As}$, with effective mass $0.1m_0$, and the contacts and the well made of GaAs, with effective mass $0.067m_0$. The second case is realized with χ of Eqs. (31) and (32) being a function of the coordinate x along the structure, say $\chi(x)$, chosen to produce a potential of a desired shape, for instance, parabolic [16,17]. The steps are introduced as a calculational intermediate. The effective mass is also changing with position.

Calculations were done previously for a double-barrier potential, with different masses and in the presence of a field [18]. The matching condition was taken the same as in the field-free case. We observed that the sum of all transmission and reflection probabilities was not summing exactly to one. It is this kind of defect that motivated the present study.

Our two examples are the scattering of an electron on a potential-free region, but with a sector-dependent effective mass and the scattering of an electron by a double barrier, also with a sector-dependent effective mass. In the two cases the particle interacts with an oscillating field. This field has an amplitude large enough to produce transitions either in reflection or in transmission with a large number of exchanged quanta.

(a) An example with variable mass and no potential change. Although this situation is not compatible with the two relations given by Eqs. (31) and (32), it is interesting to realize that a change in mass alone can accelerate or decelerate the particle, and, therefore, be the source for energy exchanges between the particle and the field. We consider two sectors of width 20 Å, with mass $0.09m_0$ enclosing a sector of width 80 Å with mass $0.067m_0$. The mass is also $0.067m_0$ in the two asymptotic regions. The amplitude of the oscillating electric field is 2×10^{-5} a.u., so that the intensity is 1.4×10^{7} W/cm^2. The energy of the incident electron is 110 meV. The frequency of the field is 50 meV. Table I shows the transmission and reflection probabilities with the sector wave functions being either those of the reduced velocity gauge [Eq. (22)] or of the velocity gauge [Eq. (24)]. Table II gives the sum of all probabilities in the different possible options: choice of gauge and field-dependent modification of the matching condition [Eq. (10)]. This is done for two values of the maximum number of exchanged quanta: $N=15$ and $N=30$. The results in the reduced velocity gauge are satisfactory for two reasons. (i) the probabilities decrease strongly as the number of absorbed photons increases, so that convergence with respect to the number of channels is achieved. (ii) The sum of all probabilities is one to a very good approximation. It is just the opposite for the velocity gauge results: no convergence, no fulfilment of the summation rule. Let us insist at this point that the usual argument about the invariance of results with respect to the choice of gauge does not apply here, because in the effective mass approximation to the real problem the A^2 term of the Hamiltonian cannot be eliminated with a sector-independent unitary operator.

(b) An example with variable mass and a double barrier. The potential in the two sectors with mass $0.09m_0$ is raised to the value 250 meV, so that the structure is now a double barrier. All other parameters remain the same. We give only the sums of all probabilities for two values of N: 15 and 30.

TABLE I. Transition probabilities for a particle meeting a region of zero potential, but with sector-dependent masses. Two sectors of width 20 Å with effective mass $0.09m_0$ enclose a sector of width 80 Å with mass $0.067m_0$, which is also the mass in the left and right asymptotic regions. The incident energy is 110 meV, the quantum 50 meV, and the amplitude of the electric field 2×10^{-5} a.u. T_n or R_n are transmission or reflection probabilities with emission (n negative) or absorption (n positive) of n quanta. v denotes results with sector functions written in the velocity gauge (with the A^2 term), while $\tilde{v}$ corresponds to calculations with sector functions in the reduced velocity gauge (without the A_2 term). Maximum number of absorbed photons: 15. All channels with $n<-2$ are closed. Parentheses are powers of 10.

Probability	v	$\tilde{v}$	Probability	v	$\tilde{v}$
T_{-2}	0.666 799 84(−4)	0.440 928 99(−4)	R_{-2}	0.176 826 00(−1)	0.141 143 38(−1)
T_{-1}	0.496 267 04(−2)	0.294 683 66(−2)	R_{-1}	0.985 462 65(−3)	0.544 958 03(−3)
T_0	0.924 028 09(+0)	0.937 085 60(+0)	R_0	0.280 662 08(−3)	0.405 441 19(−3)
T_1	0.396 952 53(−2)	0.224 024 35(−2)	R_1	0.320 305 16(−3)	0.235 828 39(−3)
T_2	0.576 507 75(−3)	0.404 831 58(−3)	R_2	0.560 501 10(−3)	0.377 567 28(−3)
T_3	0.259 790 72(−3)	0.130 995 65(−3)	R_3	0.654 691 76(−2)	0.712 516 02(−2)
T_4	0.555 954 18(−4)	0.408 149 91(−4)	R_4	0.134 632 76(−1)	0.143 257 91(−1)
T_5	0.820 788 34(−5)	0.110 239 39(−4)	R_5	0.108 459 66(−1)	0.120 121 35(−1)
T_6	0.785 447 22(−4)	0.237 465 38(−5)	R_6	0.511 507 85(−2)	0.575 040 96(−2)
T_7	0.203 612 67(−3)	0.403 531 23(−6)	R_7	0.159 722 61(−2)	0.177 762 47(−2)
T_8	0.104 254 78(−3)	0.560 628 55(−7)	R_8	0.255 210 51(−3)	0.369 615 20(−3)
T_9	0.191 421 92(−3)	0.574 850 75(−8)	R_9	0.948 860 44(−4)	0.500 576 87(−4)
T_{10}	0.561 256 03(−2)	0.161 557 69(−8)	R_{10}	0.119 218 69(−3)	0.363 250 66(−5)
T_{11}	0.989 673 08(−3)	0.275 748 64(−10)	R_{11}	0.913 639 19(−4)	0.507 008 46(−7)
T_{12}	0.116 673 76(−3)	0.625 468 03(−10)	R_{12}	0.437 091 85(−3)	0.530 163 96(−7)
T_{13}	0.819 235 93(−3)	0.288 719 88(−9)	R_{13}	0.134 436 56(−2)	0.396 115 20(−7)
T_{14}	0.122 445 14(−1)	0.546 804 94(−9)	R_{14}	0.654 487 75(−2)	0.166 490 35(−7)
T_{15}	0.593 356 68(−3)	0.268 596 32(−9)	R_{15}	0.612 848 24(−2)	0.269 774 70(−8)

The conclusions drawn from Table II indicate again an obvious superiority of the reduced velocity gauge. Increasing the number of channels in the velocity gauge leads to a diverging sum of probabilities.

As for the effect of the new matching conditions it must be indicated that with the changes of mass that are met in practical cases, the total transmissivity or reflectivity can be affected by up to 5%. Much larger changes are observed for some probabilities corresponding to particular values of the number of exchanged quanta. For instance, the probability T_2, which in the second column of Table I has the value $\sim$0.4048(−3) goes down to $\sim$0.1965(−3) when the matching is done without the field correction.

Very similar conclusions are reached when a bias potential is applied. The sector wave functions become linear combinations of Airy functions with a time-dependent argument [7,18]. Lack of convergence with respect to N is observed again when the sector functions are written is the velocity gauge. Accurate fulfilment of the sum rule is obtained only in the reduced velocity gauge.

V. CONCLUSIONS

We have examined how the matching conditions to be obeyed by a time-dependent wave function at a potential and mass discontinuity are to be modified to ensure continuity of current when the particle interacts with an oscillating electric field. This discussion does not imply a choice of gauge. In the application made to the transition probabilities of a system having the usual parameters met in the study of nanostructures, we remain with an open question: the reduced velocity gauge appears to be appropriate both from the point

TABLE II. Sum of transition probabilities with different options for the matching: $\tilde{v}$ and v stand for sector functions in reduced velocity and velocity gauges (that is, without and with the A^2 term). *cm* and *ucm* stand for corrected and uncorrected matching, with reference to the presence or absence of $f(t)$ in Eq. (10). N is the maximum number of exchanged quanta. The first two lines concern the zero potential [case (a) of the text], while the next two lines concern a double barrier [case (b) of the text].

N	$\tilde{v}+cm$	$v+cm$	$\tilde{v}+ucm$	$v+ucm$
15	1.000 0000	1.027 2944	1.027 2236	1.061 6847
30	1.000 0000	2.166 6935	1.027 2236	2.726 4120
15	0.999 999 98	1.011 0517	0.958 871 45	0.968 165 87
30	1.000 0000	32.647 374	0.958 871 46	9.140 2090

of view of convergence with respect to the number of exchanged quanta and the requirement about the sum of all probabilities. This is a curious result, since no unitary operator can be written to eliminate the A^2 term in all sectors simultaneously. However, it must be stressed that the change of gauges is not introduced at the level of the primitive Hamiltonian with the electrons and the nuclei (where invariance of any observable is easily proved), but with the effective-mass Hamiltonian that is the result of a very elaborate set of operations [19].

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[1] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), Chap 6.
[2] C. Cohen-Tannoudji, C. Diu, and F. Laloe, *Quantum Mechanics* (Hermann/Wiley, Paris, 1977).
[3] G. Bastard, Phys. Rev. B **24**, 5693 (1981).
[4] D. J. BenDaniel and C. B. Duke, Phys. Rev. **152**, 683 (1966).
[5] Ph. Stehle, *Quantum Mechanics*, (Holden-Day, San Francisco, 1966).
[6] R. A. Sacks and A. Szöke, Phys. Rev. A **40**, 5614 (1989).
[7] J. Z. Kaminski, Z. Phys. D: At., Mol. Clusters **16**, 153 (1990).
[8] S. Varró and F. Ehlotzky, J. Opt. Soc. Am. B **7**, 537 (1990).
[9] A. S. Fearnside, R. M. Potvliege, and R. Shakeshaft, Phys. Rev. A **51**, 1471 (1995).
[10] R. Lefebvre, J. Mol. Struct.: THEOCHEM **493**, 117 (1999).
[11] R. Tsu and L. Esaki, Appl. Phys. Lett. **22**, 562 (1972).
[12] M. G. Rozman, P. Reineker, and R. Tehver, Phys. Rev. A **49**, 3310 (1994).
[13] C. Pérez del Valle, R. Lefebvre, and O. Atabek, Phys. Rev. A **59**, 3701 (1999).
[14] D. K. Ferry and S. M. Goodnick, *Transport in Nanostructures* (Cambridge University Press, Cambridge, 1997).
[15] S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[16] R. C. Miller, A. C. Gossard, D. A. Kleinman, and O. Munteanu, Phys. Rev. B **29**, 3740 (1984).
[17] S. Sen, F. Capasso, A. C. Gossard, R. A. Spah, A. L. Hutchison, and S. N. G. Chu, Appl. Phys. Lett. **51**, 1428 (1987).
[18] R. Lefebvre, Int. J. Quantum Chem. **80**, 110 (2000).
[19] G. Bastard, J. A. Brum, and R. Ferreira, Solid State Phys. **44**, 229 (1991).