Quantum-mechanical evolution of real-space transfer

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A rigorous quantum-mechanical treatment of the dynamical evolution of electronic real-space transfer from a quantum well is presented, based on the density-matrix theory. A continuous electron dynamical evolution (not an abrupt collision) corresponding to a phonon absorption is analyzed here. From the evaluation of the lowest-order correction to the unperturbed density matrix, the spatial and momentum distributions can be obtained. Results will also be shown for the Wigner and Husimi functions, and it will be discussed how the present results can be used for a semiclassical modeling of real-space transfer in a Monte Carlo simulation of this effect.

I. INTRODUCTION

When electrons of a two-dimensional (2D) gas confined in a quantum well (QW) are heated up by an applied electric field, they can gain enough energy to overcome the confining potential barrier and leave the well. This phenomenon, known as real-space transfer (RST), is very important for its relevant effects on the conduction properties of many quasi 2D devices.[1,2] Usually RST takes place at the actual bias conditions used both in Si-based and in GaAs-based devices. From the theoretical point of view, however, it is very hard to rigorously include this quantum effect in a semiclassical Monte Carlo (MC) simulation. The problem is not trivial since it involves basic physical concepts and the fundamental approximations in the semiclassical description of electron transport. In traditional semiclassical transport theory, in fact, the Fermi golden rule is used to obtain a transition probability to a final state with a well-defined energy. An important question then arises as to where an electron with a given final energy and momentum is located in space soon after a collision that releases the carrier by giving it a normal-direction energy higher than the barrier height.

In the conventional quantum framework the above question has little significance. The final state is an extended state, and the electron can be located anywhere within the sample according to the amplitudes of the wave function within or outside the well, even though it seems physically intuitive that shortly after the transition the electron should still be around the well.

A quantum theory of this process is developed here with the density-matrix formalism, and quantum functions such as the Wigner function (WF) and the Husimi function (HF) are also evaluated within the same theoretical framework. Although rigorously defined in a full quantum theory of transport, such functions contain the kind of information that can be appropriately transferred to a semiclassical approximation.

A continuous dynamical evolution (not an abrupt collision) associated with a phonon interaction is described here as an important example of the application of the method. The initial condition of the system at time t_o consists of an electron in a confined state; as time increases, owing to the phonon interaction, the electron can occupy states above the confining potential with an energy spread that decreases with time, according to the uncertainty relation. At very short times the superposition of states yields a space probability density concentrated around the well and a very broad distribution in $\mathbf{k}$ space around the energy-conserving value. At longer times only states with energies closer to the conservation energy are appreciably occupied, and the electron can be located further away from the well.

This subject is developed in the following sections as follows. Section II presents a summary of the theoretical approach. In Sec. III, numerical results will be shown for the position and momentum distributions as functions of time, for physical situations of interest in practical applications, obtained from the density matrix. Two cases particularly important for their broad range of applications are considered here: electrons moving in a "model" Si well and in a GaAs-$Al_xGa_{1-x}As$-GaAs well. Furthermore, results for Wigner and Husimi distributions will be also shown in Sec. IV. Section V summarizes the main results of the paper.

II. PHYSICAL SYSTEM AND THEORETICAL APPROACH

We start, in our theoretical development, with the density-matrix formalism,[3] from the evolution equation of a state $|\Psi(t)\rangle$ of our physical system. If the Hamiltonian operator $\mathbf{H}$ can be written as the sum of an unperturbed term $\mathbf{H}_o$ and a perturbation $\mathbf{H}'$, then we have, in the Schrödinger picture

$$|\Psi(t)\rangle = \mathbf{U}_o(t,t_o)|\Psi(t_o)\rangle + \int_{t_o}^{t} \mathbf{U}_o(t,t')\mathcal{H}'|\Psi(t')\rangle\, dt' \,, \quad (1)$$

where $\mathbf{U}_o(t,t_o)$ is the unperturbed evolution operator, and $\mathcal{H}' = \mathbf{H}'/i\hbar$. In our case, $\mathbf{H}_o$ describes the electrons in the well profile and the free phonons, and $\mathbf{H}'$ is due to electron-phonon interaction ($\mathbf{H}' = \mathbf{H}_a + \mathbf{H}_e$, $\mathbf{H}_a = \mathbf{H}_e^\dagger$, where "$a$" and "$e$" refer to absorption and emission, respectively).

The first-order correction to the unperturbed state is then given by

$$|\Delta\Psi(t)\rangle = \int_{t_o}^{t} \mathbf{U}_o(t,t')\mathcal{H}'\mathbf{U}_o(t',t_o)|\Psi(t_o)\rangle\, dt' \,. \tag{2}$$

We want to study a physical process where a phonon has been absorbed, so that we need to write the correction to the density matrix which describes the phonon bath in a diagonal state with a phonon of energy $\hbar\omega_q$ missing with respect to the initial state. Assuming only one phonon mode ($\mathbf{q}$, ω_q) with occupation number n_q, we will use in the following the usual expression for the optical-phonon interaction Hamiltonian[4] relative to the mode $\mathbf{q}$

$$\mathbf{H}' = i\hbar F(q)(b_q e^{i\mathbf{qr}} - b_q^\dagger e^{-i\mathbf{qr}}) = \mathbf{H}_a + \mathbf{H}_e \tag{3}$$

(F is a real function that depends on the electron-phonon interaction mechanism).

For the purpose of this paper, concerned with the location of an electron after a real-space transition induced by a phonon absorption, we are interested in the lowest contribution to the density matrix on a time scale of the order of the electron-phonon collision time ($\approx$ 100 fs). This correction is given by

$$\begin{aligned}\Delta\rho(t) &= |\Delta\Psi(t)\rangle\langle\Delta\Psi(t)| \\ &= -\int_{t_o}^{t} \mathbf{U}_o(t,t_1)\mathcal{H}'_a\mathbf{U}_o(t_1,t_o)|\Psi(t_o)\rangle dt_1 \\ &\quad\times\int_{t_o}^{t}\langle\Psi(t_o)|\mathbf{U}_o^\dagger(t_2,t_o)\mathcal{H}'^\dagger_a\mathbf{U}_o^\dagger(t,t_2)\, dt_2 \,.\end{aligned} \tag{4}$$

Second-order terms due to second-order corrections of the state vector correspond to virtual processes (scattering out in semiclassical terms),[4] and they are of no interest in the present treatment.

In our calculations we assume that at the beginning of the interaction the electron is in its ground state, but the theory can be easily extended to the case of an initial excited state.

Then let $|o\mathbf{K}n_q\rangle$ be the imitial state of the whole system, where $\mathbf{K}$ indicates the electron 2D momentum parallel to the well plane and ω_K the corresponding energy, and o the ground state of the particle in the QW with energy $\hbar\omega_o$. Finally, after some substitutions in Eq. (4) we obtain, for an absorption process,

$$\begin{aligned}\Delta\rho(t) &= -\int_{t_o}^{t} dt_1 \int_{t_o}^{t} dt_2 \mathbf{U}_o(t,t_1)\mathcal{H}'_a\mathbf{U}_o(t_1,t_o)|o\mathbf{K}n_q\rangle\langle o\mathbf{K}n_q|\mathbf{U}_o(t_o,t_2)\mathcal{H}'^\dagger_a\mathbf{U}_o(t_2,t) \\ &= F^2(q)\int_{t_o}^{t} dt_1 \int_{t_o}^{t} dt_2 e^{-i(\omega_o+\omega_K+\omega_{n_q})(t_1-t_2)}\mathbf{U}_o(t,t_1)\sqrt{n_q}e^{i\mathbf{qr}} \\ &\quad\times|o\mathbf{K}n_q-1\rangle\langle o\mathbf{K}n_q-1|\sqrt{n_q}e^{-i\mathbf{q}\cdot\mathbf{r}}\mathbf{U}_o(t_2,t) \,.\end{aligned} \tag{5}$$

By including the identity operator written as the sum of the projection operators over the eigenstates $|n\mathbf{K},n_q\rangle$ of the system, we have

$$\begin{aligned}\Delta\rho(t) &= F^2(q)n_q\sum_{nm}\sum_{K',K''}\int_{t_o}^{t} dt_1\int_{t_o}^{t} dt_2 e^{-i(\omega_o+\omega_K+\omega_{n_q})(t_1-t_2)}e^{-i(\omega_n+\omega_{K'}+\omega_{n_q-1})(t-t_1)} \\ &\quad\times|nK',n_q-1\rangle M_{no}(q)\langle\mathbf{K}'|e^{i\mathbf{Q}\cdot\mathbf{R}}|\mathbf{K}\rangle M_{om}(-q)\langle\mathbf{K}|e^{-i\mathbf{Q}\cdot\mathbf{R}}|\mathbf{K}''\rangle\langle mK'',n_q-1| \,.\end{aligned} \tag{6}$$

In the above equation, $\mathbf{Q}$ is the initial phonon wave vector along the plane of the well, the labels n and m are for the excited itinerant eigenstates including the well potential, and the labels $\mathbf{K}$ and $\mathbf{K}'$ are for the continuum of dynamical states parallel to the well planes. Furthermore, $M_{no}(q) = \langle n|e^{iq_z z}|o\rangle$ are the matrix elements of the phonon-field factor $\exp(iq_z z)$ between the initial electron state and the excited itinerant electron states n (the potential well has been assumed to be in the z direction). In the sums over n and m present in Eq. (6) we neglected the contribution of the (few) excited bound states of the well, which is negligible compared to the other contributions coming from itinerant states.

Furthermore, we have

$$\langle\mathbf{K}|e^{i\mathbf{Q}\cdot\mathbf{R}}|\mathbf{K}''\rangle = \delta_{K-K''+Q} \,. \tag{7}$$

As it regards the phonon part, taking the trace over phonon states

$$\sum_{n_q'}|n_q'\rangle n_q'\langle n_q'| \tag{8}$$

we obtain the Planck function $\langle n_q\rangle$, and evaluating the two time integrals, we finally obtain the contribution to the density matrix due to a phonon absorption at time t

$$\begin{aligned}\Delta\rho(t) &= F^2(q)\langle n_q\rangle\sum_{nm}M_{no}(q)M_{om}(-q)\mathcal{T}(\omega_n,t) \\ &\quad\times\mathcal{T}^*(\omega_m,t)|n\mathbf{K}+\mathbf{Q}\rangle\langle m\mathbf{K}+\mathbf{Q}| \,,\end{aligned} \tag{9}$$

where

$$\mathcal{T}(\omega_n) = e^{-i\omega_n(t-t_o)}\frac{e^{-i(\omega_f-\omega_n)(t-t_o)}-1}{(\omega_f-\omega_n)} . \quad (10)$$

In the above equation $\hbar\omega_f = \hbar(\omega_o+\omega_K+\omega_q-\omega_{K+Q})$ is the residual normal-direction energy of the electron under energy-conservation conditions.

Since the dynamics in the well plane are separated from that normal to the well, from the above expression the probability density $f(z)$ of electron position [or momentum $P(k_z)$] normal to the well, associated with $\Delta\rho$ in Eq. (9), can be obtained by taking z (or k_z) diagonal elements

$$\begin{aligned} f(z) &= \langle z|\Delta\rho|z\rangle \\ &= F^2(q)\langle n_q\rangle \sum_{nm} M_{no}(q)M_{om}(-q)\mathcal{T}(\omega_n,t)\mathcal{T}^*(\omega_m,t)\psi_n(z)\psi_m^*(z) \\ &= F^2(q)\langle n_q\rangle \left|\sum_n M_{no}(q)\mathcal{T}(\omega_n,t)\psi_n(z)\right|^2 , \end{aligned} \quad (11)$$

$$\begin{aligned} P(k_z) &= \langle k_z|\Delta\rho|k_z\rangle \\ &= F^2(q)\langle n_q\rangle \sum_{nm} M_{no}(q)M_{om}(-q)\mathcal{T}(\omega_n,t)\mathcal{T}^*(\omega_m,t)\langle k_z|n\rangle\langle m|k_z\rangle \\ &= F^2(q)\langle n_q\rangle \sum_{nm} M_{no}(q)M_{om}(-q)\mathcal{T}(\omega_n,t)\mathcal{T}^*(\omega_m,t)\int dz\ \psi_{k_z}^*(z)\psi_n(z)\int dz'\ \psi_m^*(z')\psi_{k_z}(z') \\ &= F^2(q)\langle n_q\rangle \left|\sum_n M_{no}(q)\mathcal{T}(\omega_n,t)\int dz\psi_{(k_z)}^*(z)\psi_n(z)\right|^2 . \end{aligned} \quad (12)$$

The results in Eqs. (11) and (12) are thus the modulus squared of the wave function of the electron system in the z and k_z representation, respectively.

The Wigner function can also be obtained from the knowledge of the density matrix.[5] For a pure state the WF is defined as the Weyl-Wigner transformation of the density-matrix operator $\Delta\rho(t) = |\Delta\Psi(t)\rangle\langle\Delta\Psi(t)|$

$$f_W(q,p) = \frac{1}{2\pi\hbar}\int d\eta\ e^{\frac{i\eta p}{\hbar}}\langle q-\tfrac{1}{2}\eta|\Psi\rangle\langle\Psi|q+\tfrac{1}{2}\eta\rangle \quad (13)$$

and in the wave-function representation

$$f_W(q,p) = \frac{1}{2\pi\hbar}\int d\eta\ e^{\frac{i\eta p}{\hbar}}\Psi^*(q+\tfrac{1}{2}\eta)\Psi(q-\tfrac{1}{2}\eta) . \quad (14)$$

An intuitive physical meaning of the WF is contained in its definition: it expresses the p component of the amount of correlation of the wave function around the q point. Since the WF contains phase information from the wave function, it can also assume negative values and cannot be interpreted as a "quantum distribution function." Furthermore, it can be different from zero at q points where the wave function itself is zero. Nevertheless, the WF becomes a valid probability function if integrated over q or over p, and it can be used to evaluate averages of observable operators.[5]

There are other methods that allow extraction of "distribution functions" with special properties from the density operator, by applying transformations different from the Weyl-Wigner transform. One important example of a *positive-definite* function is the Husimi function.[5] The HF can also be obtained from the WF as[6]

$$f_H(q,p) = \frac{1}{\pi\hbar}\int dq'\int dp' e^{-\frac{(q-q')^2}{\alpha}} \times e^{-\frac{\alpha(p-p')^2}{\hbar^2}} f_W(q',p') . \quad (15)$$

Here α is a smearing parameter. It can be proven that the HF is positive definite, it is often used in the description of harmonic oscillators and, hence, modes of the electromagnetic field.[5]

For further development of the calculation we need to explicitly make a choice for the form of the potential well along the z direction and for the electronic localized and extended states relative to this well.

III. RESULTS FOR THE DENSITY MATRIX

Numerical results will be presented for a model square well of width L and depth V_o. The electron at $t = 0$ is supposed to be in the ground state of the well and, for $t > 0$, it interacts with a phonon mode of energy $\hbar\omega_q$ and wave vector $\mathbf{q}$. Suitable values have been chosen for physical quantities to represent the physical cases of Si-based QW and GaAs-Al_xGa_{1-x}As-GaAs QW. The list of these parameters is given in Table I.

In order to evaluate $f(z) = \Delta\rho_{zz}$ from Eq. (11) in the previous section we must specify the form of the complete set of wave functions $\psi_m(z)$ describing the electron 1D states in the well. For this calculation the extended itinerant states with energy $\varepsilon > V_o$ have been chosen as

TABLE I. List of parameters used in the calculations of RST in Si structure (upper line) and GaAs structure (lower line). Here L is the well length, V_o the well depth (V=0 at the bottom of the well); m^* is the electron effective mass, $T_{\rm ph}$ is the phonon equivalent temperature, q_z is the z component of the phonon wave vector, and $\hbar\omega_f$ the energy of the final state of the electron.

Structure	L (A)	V_o (eV)	m^*	$T_{\rm ph}$ (K)	$q_z(m^{-1})$	$\hbar\omega_f$ (eV)
Si	50	1	0.295	500	2.9×10^9	1.1
GaAs	30	0.55	0.067	410	1.0×10^9	0.6

even and odd functions. Substituting for the label n a more appropriate continuous label k_z, we used the following functions:

$$\psi_{k_z}^{(+)}(z) = \begin{cases} B\sin(k'z+\phi^{(+)}) & , -a/2 < z < -L/2 \\ A^{(+)}\cos(k_z z) & , \quad -L/2 < z < L/2 \\ -B\sin(k'z-\phi^{(+)}) & , \quad a/2 > z > L/2 \, , \end{cases} \tag{16}$$

$$\psi_{k_z}^{(-)}(z) = \begin{cases} B\sin(k'z+\phi^{(-)}) & , \quad -a/2 < z < -L/2 \\ A^{(-)}\sin(k_z z) & , \quad -L/2 < z < L/2 \\ B\sin(k'z-\phi^{(-)}) & , \quad a/2 > z > L/2 \, . \end{cases} \tag{17}$$

Here k' and k_z are the wave vectors of the stationary state outside and inside the well, respectively, and the constants A, B, and ϕ are fixed by imposing the usual condition of continuity of the function and its derivative at $z = \pm L/2$. The normalization condition has been imposed within a box of length $a \gg L$ ($1000A$ in the calculation).

The wave function of the ground state must be symmetric and without nodes. It can be written as

$$\psi_o(z) = \begin{cases} A_1 e^{\kappa_o z} & , \quad -a/2 < z < -L/2 \\ A_o \cos k_o z & , \quad -L/2 < z < L/2 \\ A_1 e^{-\kappa_o z} & , \quad a/2 > z > L/2 \, , \end{cases} \tag{18}$$

where κ_o and k_o are the wave vectors outside and inside the well, respectively.

Figures 1 and 2 show the probability $f(z)$ of finding the electron around the well after the onset of the interaction with an optical phonon as a function of the z coordinate, for the Si structure and GaAs structure, respectively. The observation time is $t = 100$ fs after the initial condition.

The probability of finding the particle outside the well is larger for $z > 0$ because of the orientation of the phonon mode.

Figure 3 shows the same quantity for increasing times up to 200 fs for the GaAs case. It is seen that the probability of finding the particle outside the well increases with time. Furthermore, the two leading edges of the function $f(z)$ for $z > 0$ and $z < 0$ correspond to the distances traveled at the assumed time t, forwards and backwards along the z axis by a classical free particle with a normal energy component corresponding to the energy-conserving value.

With increasing time, the distribution $f(z)$ tends to fill the space from the well to the position of its leading edge. This corresponds to the use of the second-order perturbation by the electron-phonon interaction $\mathbf{H}'$ in Eq. (6), the lowest applicable order, which means that the itinerant states are filled from a state (the ground state in the well) which effectively remains occupied.

For the evaluation of $P(k_z)$ in Eq. (12) the states $\psi_{k_z}(z)$ not confined inside the well have been chosen as the linear combinations of the previous functions [see Eq. (16) and Eq. (17)] which behave as traveling waves inside the well

$$\begin{aligned} \psi_{k_z}(z) &= \frac{1}{\sqrt{A^{(+)2}+A^{(-)2}}}\left[A^{(-)}\psi_{k_z}^{(+)}(z) + iA^{(+)}\psi_{k_z}^{(-)}(z)\right] \\ &= \frac{1}{\sqrt{A^{(+)2}+A^{(-)2}}} \begin{cases} B[A^{(-)}\sin(k'z+\phi^{(+)}) + iA^{(+)}\sin(k'z+\phi^{(-)})], & -a/2 < z < -L/2 \\ A^{(+)}A^{(-)}e^{ik_z z}, & -L/2 < z < L/2 \\ B[-A^{(-)}\sin(k'z+\phi^{(+)}) + iA^{(+)}\sin(k'z+\phi^{(-)})], & a/2 > z > L/2 \, , \end{cases} \end{aligned} \tag{19}$$

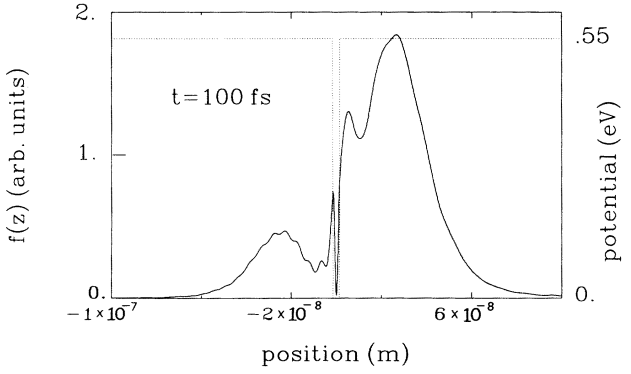

FIG. 1. Probability of finding the electron outside the well as a function of the z coordinate at $t = 100$ fs (left vertical axis, continuous line) for the Si structure. The shape of the potential well (right vertical axis, dotted line) is also shown.

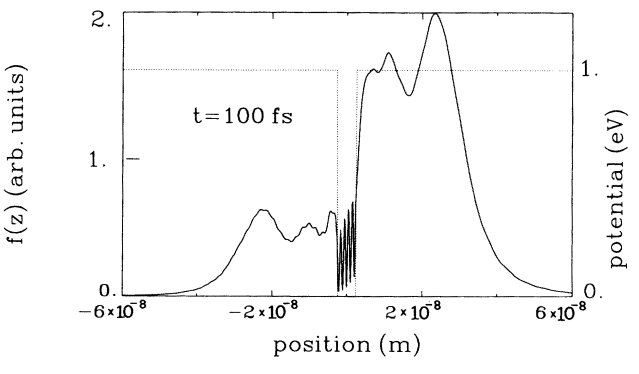

FIG. 2. Probability of finding the electron outside the well as a function of the z coordinate at $t = 100$ fs (left vertical axis, continuous line) for the GaAs structure. The shape of the potential well (right vertical axis, dotted line) is also shown.

$$\psi_{-k_z}(z)= \frac{1}{\sqrt{A^{(+)2}+A^{(-)2}}}[A^{(-)}\psi^{(+)}_{k_z}(z) - iA^{(+)}\psi^{(-)}_{k_z}(z)]$$
$$= \frac{1}{\sqrt{A^{(+)2}+A^{(-)2}}} \begin{cases} B[A^{(-)}\sin(k'z+\phi^{(+)}) - iA^{(+)}\sin(k'z+\phi^{(-)})] , & -a/2 < z < -L/2 \\ A^{(+)}A^{(-)}e^{-ik_z z} , & -L/2 < z < L/2 \\ B[-A^{(-)}\sin(k'z+\phi^{(+)}) - iA^{(+)}\sin(k'z+\phi^{(-)})] , & a/2 > z > L/2 . \end{cases} \quad (20)$$

Figures 4 and 5 show, at the same times as in Fig. 3, the probability $P(k_z)$, as a function of k_z, of finding the electron in the final states of Eq. (19) and Eq. (20) for the Si case and the GaAs case, respectively. It is seen that the distribution narrows at larger times because of the approaching of the energy-conservation condition. Correspondingly, the space distribution is broadened, as shown in Fig. 3, according to the uncertainty principle.

It is interesting to notice that $P(k_z)$ exibits a maximum around a certain value of k_z (which can be positive or negative according to the direction of the phonon wave vector), and a much smaller maximum at the opposite k. For the case of Si, this secondary maximum is hardly observed, while it is well shown for the case of GaAs. This fact can be explained if we consider the following. Momentum is not conserved for our system, owing to the presence of the well potential. However, the matrix elements M evaluated for the basis functions in Eq. (19) and Eq. (20)

$$M \propto \int dz\psi_o[\cos(qz) + i\sin(qz)] \times[A^{(-)}\psi^{(+)}_{k_z}(z) \pm iA^{(+)}\psi^{(-)}_{k_z}(z)] , \quad (21)$$

are found to have their maximum values, as would be expected, around the k which satisfies the "classical" conservation law.[7] Remembering that the momentum distribution for the ground state of the well is centered around $k = 0$, we have that the maximum of M should be around $k \sim q_z$. This is shown in Fig. 6. Because of this term, transitions close to momentum conservation would be favored.

Furthermore, the time factors present in $P(k_z)$ (expressing the "quasi" energy conservation at short times) are oscillatory functions of k_z strongly peaked at the (symmetrical) k values associated with energy conservation for these physical conditions, as shown in Fig. 6 for the case of Si. This fact favors transitions to two well-defined degenerate plane-wave states inside the well traveling in opposite directions.

The net effect of the two factors is a bump at k_z values where both terms are significantly different from zero, and, correspondingly, one of the two energy-conserving states (the one with k_z parallel to the phonon wave vector q_z) is much more favored compared to the opposite one. For this reason, in Figs. 4 and 5, $P(k_z)$ is different from zero mainly around a positive k_z.

IV. RESULTS FOR THE WIGNER AND HUSIMI FUNCTIONS

Figures 7 and 8 show the WF at a time $t = 100$ fs, for the Si and GaAs structure, respectively, obtained from the density matrix contribution in Eq. (9), as a function of the position and momentum orthogonal to the well. In contrast to Figs. 4 and 5, where k labels the eigenfunctions of the well potential, here owing to the definition of the WF in Eq. (13) $k = p/\hbar$ represents the eigenvalue of the momentum operator.

It is interesting to notice that the momentum probability distribution, as obtained from the WF, shows two peaks, associated with the bumps of the 3D function shown in Figs. 7 and 8, at the positive and negative symmetrical values of the momentum corresponding to energy conservation. The peak at the negative k is ab-

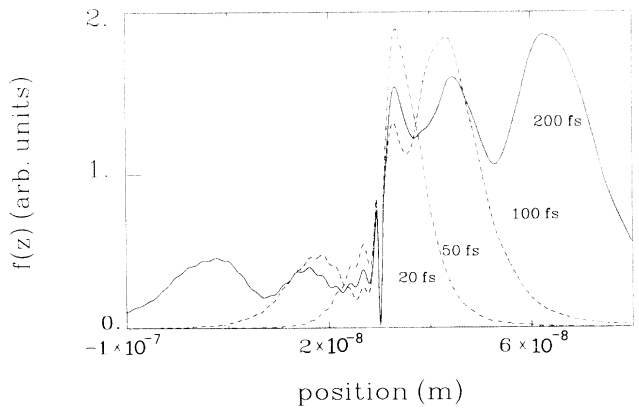

FIG. 3. Probability of finding the electron outside the well as a function of the z coordinate at different times for the Si structure.

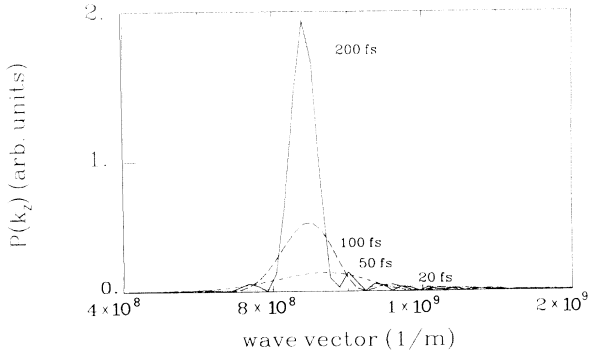

FIG. 4. Probability of finding the electron outside the well as a function of the z coordinate at different times for the GaAs structure.

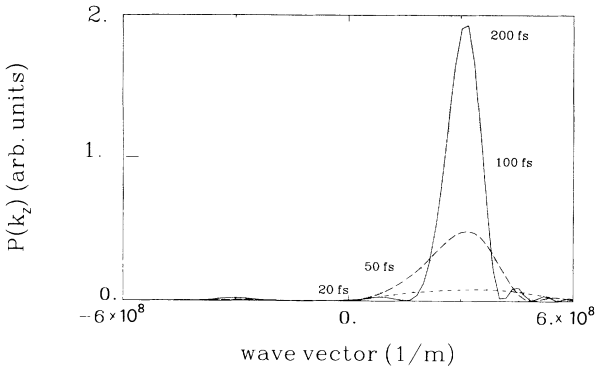

FIG. 5. Probability of finding the electron in a final k state with the k_z value inside the well (see text) at different times for the GaAs structure.

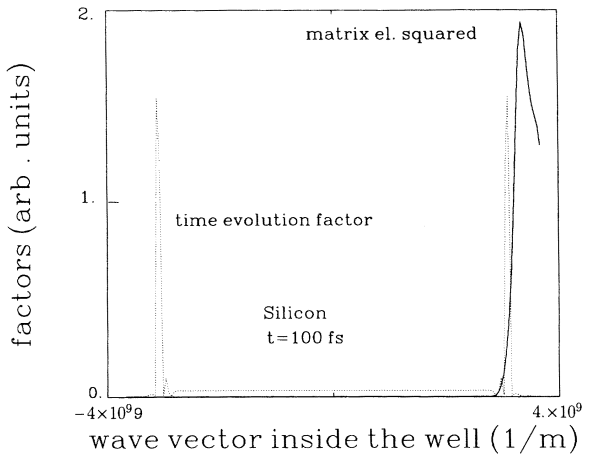

FIG. 6. Squared modulus of the matrix elements M evaluated for the basis functions given in Eq. (19) and Eq. (20) (continuous line) and of the time evolution factor $\mathcal{T}(\omega_n, t)$ (dotted line) in Eq. (12) as functions of the wave vector k_z inside the well (see text). Here we considered $t = 100$ fs and $q_z = 2.9 \times 10^9$ m^{-1}.

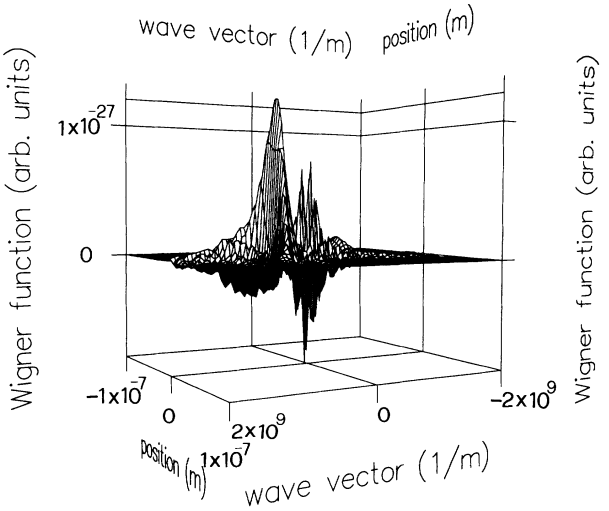

FIG. 7. Wigner distribution as a function of position and momentum orthogonal to the well at $t = 100$ fs after the beginning of a quantum phonon-absorption process for the Si structure (same case as in Fig. 1).

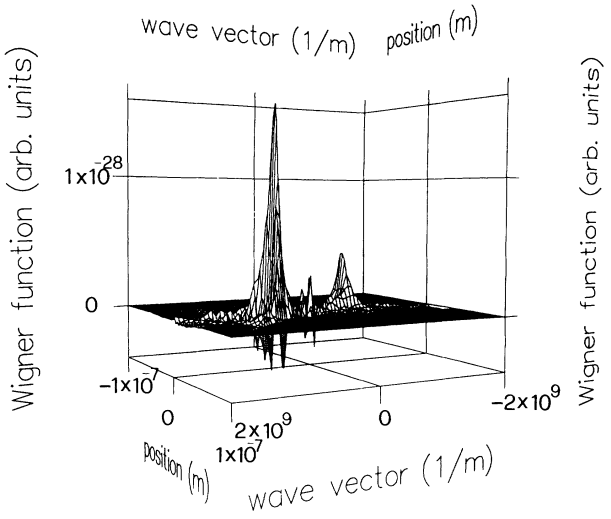

FIG. 8. Wigner distribution as a function of position and momentum orthogonal to the well at $t = 100$ fs after the beginning of a quantum phonon-absorption process for the GaAs structure (same case as in Fig. 2).

sent in the $P(k_z)$ plot, because in this last case k_z represents the particle momentum only inside the well (see discussion in the previous section). The negative peak, as obtained from the WF, is due to a quantum reflection at the barrier edge. Furthermore, strong oscillations in the WF are observed in the spatial region of the well due to the coherence of the electron states leaving the well in the two opposite directions.

Figure 9 shows as an example, the HF for the same cases as in Fig. 8. The parameter α has been chosen as $(9\text{ nm})^2$.

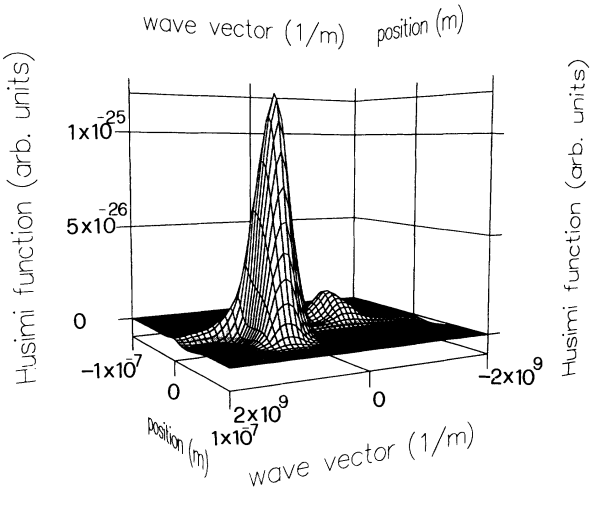

FIG. 9. Husimi distribution as a function of position and momentum orthogonal to the well at $t = 100$ fs after the beginning of a quantum phonon-absorption process for the GaAs structure obtained from the Wigner function shown in Fig. 8.

As discussed above, the HF is positive definite, and it can be used in a traditional semiclassical MC simulation as a realistic model for a "joint" position and momentum probability distribution, if RST must be taken into account in a semiclassical scheme. In this connection it can be observed that the criterion we have adopted for the choice of the smoothing parameter α is that the HF must reproduce the gross shape of the WF without the oscillations coming from the coherence properties of the quantum wave function.

V. CONCLUSIONS

A method is given based on the density-matrix formalism for the calculation of the spatial and momentum distributions of an electron which escapes a localized state in a quantum well as an effect of real-space transfer assisted by the absorption of an optical phonon. The Wigner and Husimi distributions have also been evaluated. The Husimi distribution can be a good semiclassical joint probability distribution for position and momentum in order to include real-space transfer in a traditional Monte Carlo simulation. Numerical results have been obtained for Si-based and GaAs-based structures.

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