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Decoherence and time reversibility: The role of randomness at interfaces

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The Wigner formalism is a convenient reformulation of the Schrödinger equation that allows the simulation of transient behavior of quantum systems in the presence of general boundary conditions. Recently, a Wigner Monte Carlo technique, based on particles signs, has been generalized to two-dimensional evolution problems. In this paper, we apply this technique to study the time reversibility of the quantum evolution of a wave packet colliding with a potential wall in the presence of interface roughness, elastic, inelastic, and diffusive interactions with the environment. We show that a wall surface roughness does not necessarily involve time irreversibility. The dynamics of the packet is indeed influenced, but remains coherent, until the boundaries of the system begin to absorb information from the system. Finally, it is shown that in the presence of inelastic scattering or diffusive processes, the time-reversibility of a quantum system is destroyed, whatever the shape of the wall interface is. In particular, we show that the random nature of a process, elastic or inelastic, is responsible for the appearance of quantum decoherence.
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I. INTRODUCTION

As today nanometer scaled semiconductor devices are becoming part of our everyday life, quantum transport of charged particles is gradually getting importance in the field of engineering and practical applications. Many aspects of quantum transport are still not well understood, both from an experimental and theoretical point of view. For example, as recently demonstrated, the coupling of classical boundary conditions (BCs) to stationary quantum models may lead to non-unique solutions having no physical sense.[1] Research to understand the effects of BCs on full quantum models is, as a matter of fact, still a work in progress. Many other problems related to the simulation of quantum phenomena are still open, among them is the phenomenon known as quantum decoherence. We focus on this phenomenon in the presence of open BCs.

The emergence of classical dynamics in initially pure quantum systems is a process that can be explained in terms of quantum decoherence. Indeed, when this process occurs, the coherence between the eigenstates is destroyed along with the quantum information of the system so that time reversibility cannot happen any longer. Only a few states will survive to the environment and the vast majority of the corresponding Hilbert space states is simply ignored from the physics of the quantum system. Despite this description may sound very theoretical, it is a very tangible effect that can be observed in experiments and occurs in technologically relevant situations such as in nanometer scaled devices. The study of this quantum phenomenon has practical implications. For example, it explains why certain nanodevices cannot operate at room temperature. In order to investigate these particular systems, a full quantum model must be utilized.

A good candidate for a full quantum model is the Wigner formalism which is a generalization of the time-dependent Schrödinger equation in terms of a phase-space. The model is general enough to naturally include open BCs, general initial conditions, and also the effects of lattice phonon scattering. It has been already applied to study the emergence of decoherence in a variety of situations ranging from atomic physics,[2,3] to quantum electronic transport.[4–6] In this paper, we apply the Wigner formalism to two-dimensional (2D) situations and study the quantum dynamics of the system in the presence of general random (elastic and inelastic) processes (theoretical models) in order to understand the nature of quantum decoherence and the transition to classical mechanics.

The first attempts to simulate quantum transport with the Wigner equation were based on the finite difference method which introduces some numerical problem.[7–9] The challenge is posed by the diffusion term of the Liouville operator, since the solution of the Wigner equation is rapidly oscillating around the regions of the phase space, where quantum interference is dominant. During the last decade, Monte Carlo particle models which avoid the calculation of the diffusion term were developed. Furthermore, decoherence effects of boundaries and phonon scattering can now be included at equal footing, in a similar fashion to the Boltzmann MC method, which is hardly achievable with other full quantum models.

One of these implemented MC methods introduces the concept of particle affinity,[10,11] a real number that carries the quantum information of the system. This method has shown to be successful in many aspects and has been applied to self-consistent simulations of actual nanometer sized devices. However, the required amount of computational resources precludes multi-dimensional applications. Another

model introduced the concept of signed particles, generated by the Wigner potential, which may annihilate each other in the phase-space. This method needs ergodic conditions and is relevant for stationary problems posed by BCs.[12]

Recently, this approach has been generalized to time-dependent transport determined by general boundary and initial conditions.[13] It exploits the notions of momentum quantization and indistinguishable particles. These concepts, proper to quantum mechanics, entangled with the classical notions of trajectories, particle ensemble, and particle annihilation at consecutive time steps allow implementations beyond one-dimensional evolution. Indeed, even if sophisticated computational resources are welcome, they are not imposed by this MC approach. As a matter of fact, we are able to simulate two-dimensional numerical experiments in order to study the evolution of quantum systems.[14]

In this paper, we present five numerical experiments to show how inelastic, diffusive, and random processes can trigger quantum decoherence. We interchangeably use the (equivalent) concepts of coherent regime, time reversibility, and quantum purity.[15] We start by simulating a time reversible situation consisting of a Gaussian wave packet interacting with a flat wall or, equivalently, a flat interface. This shows that the method utilized is reliable and relevant for our analysis. We then proceed by introducing roughness at the interface and show that the system is time reversible even in this case. Then, an inelastic process at a flat interface is introduced, which reduces particle energies by a constant amount. The system is shown to be time irreversible and decoherence appears. The fourth experiment consists of introducing randomness at the interface, which now removes a stochastic amount of energy from the particles. The random nature of the process affects the time reversibility of the system. These results altogether clearly show that roughness alone cannot trigger decoherence. An inelastic or diffusive (random) process is necessary to make a quantum system time irreversible. Finally, we introduce a diffusive process which randomizes the direction of the particle wave numbers while keeping their energy constant. Even in this case, the system becomes time irreversible, although the process is elastic. This result shows that the appearance of decoherence is intimately connected to the randomness of a process happening at the interface.

II. THE 2D WIGNER MONTE CARLO METHOD

The Wigner approach can be considered as a phase-space reformulation of the density matrix formalism.[16,17] The two models are theoretically equivalent. The Wigner equation reads

$$\frac{\partial f_W}{\partial t} + \frac{\hbar \mathbf{k}}{m^*} \cdot \nabla_{\mathbf{x}} f_W = Q_W[f_W], \tag{1}$$

where $f_W = f_W(\mathbf{x}, \mathbf{k}, t)$ is the unknown pseudo-distribution function (it can have negative values) defined over the phase-space $(\mathbf{x}, \mathbf{k}) = (x, y, k_x, k_y)$, m^* is the effective mass, Q_W is a functional defined as

$$Q_W[f_W](\mathbf{x}, \mathbf{k}, t) = \int d\mathbf{k}' V_W(\mathbf{x}, \mathbf{k} - \mathbf{k}', t) f_W(\mathbf{x}, \mathbf{k}, t), \tag{2}$$

and the Wigner potential is defined as

$$V_W(\mathbf{x}, \mathbf{k}, t) = \frac{1}{i\hbar 4\pi^2} \int d\mathbf{x}' e^{-i\mathbf{k}\cdot\mathbf{x}'} [V_+ - V_-], \tag{3}$$

where $V_\pm = V(\mathbf{x} \pm \frac{\mathbf{x}'}{2}, t)$ is the potential function acting over the domain. For convenience, in the following, we omit the time dependence of V_W.

This model can be rewritten exploiting the semi-discrete nature of the phase-space.[13] On one side, physical considerations show that the simulation domain for the quantum structure is bounded by an upper limit $\mathbf{L}_C = (L_C^x, L_C^y)$ known as the coherence length. This means that a discrete Fourier transform can be applied in (3). On the other side, according to the tenets of quantum mechanics, particle energy comes in quanta. This is equivalent to say that the k-space is expressed in terms of multiples of a finite quantity $\Delta\mathbf{k} = \frac{\pi}{\mathbf{L}_C}$.

Furthermore, it is possible to reformulate the semi-discrete Wigner equation in an adjoint integral form having a solution which can be written in terms of a series. In particular, if $A = A(\mathbf{x}, \mathbf{k})$ is some generic physical quantity, it is possible to express its expectation value as a series

$$\langle A \rangle = \int_0^\infty dt' \int d\mathbf{x}_i \sum_{\mathbf{m}'=-\infty}^{\infty} f_i(\mathbf{x}_i, \mathbf{m}') e^{-\int_0^{t'} \gamma(\mathbf{x}_i(y))dy} g(\mathbf{x}_i(t'), \mathbf{m}', t'), \tag{4}$$

where $f_i = f_i(\mathbf{x}, \mathbf{m})$ is the initial conditions at time 0. The function $g = g(\mathbf{x}, \mathbf{m}, t)$ is the solution of the adjoint equation which contains the quantity $A = A(\mathbf{x}, \mathbf{k})$. The details are in Ref. 13.

We report the first two terms of the series and give a physical interpretation

$$\langle A \rangle_0(\tau) = \int_0^\infty dt' \int d\mathbf{x}_i \sum_{\mathbf{m}'=-\infty}^{\infty} f_i(\mathbf{x}_i, \mathbf{m}') e^{-\int_0^{t'} \gamma(\mathbf{x}_i(y))dy} \times A(\mathbf{x}_i(t'), \mathbf{m}') \delta(t' - \tau). \tag{5}$$

From a pure mathematical MC perspective, the integrand can be considered as a product of conditional probabilities. Assuming that f_i is normalized, random points $\mathbf{x}_i, \mathbf{m}'$ at time 0 can be generated. This can be considered as an initialization of particle trajectories $\mathbf{x}_i(y)$. The exponent in the integrand is interpreted as the probability for the particle to remain in its trajectory and the scattering rate is given by the function $\gamma(\mathbf{x})$ which is defined later. If a scattering time is generated randomly (less than τ), the probability acts as a filter to the particles. Indeed, if a particle is not scattered until time τ, it contributes to $\langle A \rangle_0(\tau)$ with the value $f_i(\mathbf{x}_i, \mathbf{m}') A(\mathbf{x}_i(\tau), \mathbf{m}')$. Thus, $\langle A \rangle_0(\tau)$ is estimated by using the mean value of the N initialized particles. On the other hand, if the particle is scattered, then it does not contribute to $\langle A \rangle_0(\tau)$ but to the term $\langle A \rangle_1(\tau)$

$$\langle A\rangle_1(\tau) = \int_0^\infty dt' \int \mathrm{d}\mathbf{x}_i \sum_{\mathbf{m}'=-\infty}^{\infty} f_i(\mathbf{x}_i, \mathbf{m}')\{\gamma(\mathbf{x}_i(t'))e^{-\int_0^{t'}\gamma(\mathbf{x}_i(y))dy}\} \times \theta_D(\mathbf{x}_1)$$
$$\times \int_{t'}^{\infty} \mathrm{d}t \sum_{\mathbf{m}=-\infty}^{\infty} \left\{\frac{\Gamma(\mathbf{x}_1, \mathbf{m}, \mathbf{m}')}{\gamma(\mathbf{x}_i(t'))}\right\}\{e^{-\int_{t'}^{t}\gamma(\mathbf{x}_1(y))dy}\}A((\mathbf{x}_1(t), \mathbf{m}, t)\delta(t-\tau), \quad (6)$$

where

$$\Gamma(\mathbf{x}, \mathbf{m}, \mathbf{m}') = V_w^+(\mathbf{x}, \mathbf{m}-\mathbf{m}') - V_w^+(\mathbf{x}, -(\mathbf{m}-\mathbf{m}')) + \gamma(\mathbf{x})\delta_{\mathbf{m},\mathbf{m}'} \quad (7)$$

and $V_W^+ = V_w^+(\mathbf{x}, \mathbf{m})$ is the positive part of the Wigner function. This time a particle is initialized at $\mathbf{x}_i, \mathbf{m}', 0$ and follows the trajectory until time t' (which is the time of scattering given by the probability density in the first curly brackets). It is easy to see that the exponent is the probability to not scatter until time t', while $\gamma(\mathbf{x}_i(t'))dt'$ is the probability to scatter in the interval $[t', t'+dt']$. The particle is now in the phase-space position $\mathbf{x}_1 = \mathbf{x}_i(t'), \mathbf{m}', t'$ and the evolution continues as long as the particle remains in the simulation domain. Otherwise the domain indicator $\theta_D = \theta_D(\mathbf{x})$ changes the value from 1 to 0 and the contribution is zero. The term in the next curly bracket can be interpreted as a source of scattering from $\mathbf{m}'$ to $\mathbf{m}$ (locally in space at point $\mathbf{x}_1$ and time t'). Thus, at moment t', the particle initializes the trajectory $\mathbf{x}_1, \mathbf{m}$ and, with the probability given by the exponent in the last curly brackets, remains over the trajectory until time τ is reached: t is set to τ by the δ function provided that $t' < \tau$, otherwise the contribution is zero. In the same way, a physical interpretation of the other terms of the series can be given.

From the previous observations, a MC approach for the semi-discrete Wigner equation can now be depicted. By considering the quantity

$$\gamma(\mathbf{x}) = \sum_{\mathbf{m}=-\infty}^{+\infty} V_W^+(\mathbf{x}, \mathbf{m}) \quad (8)$$

as a normalization factor, (7) describes the generation process of two particles, with a positive and a negative sign, respectively, and the surviving initial particle with its sign due to the δ function. More specifically, an initial particle with sign s and wave-vector $\mathbf{n}$ generates, with a rate $V^+(\mathbf{l})$, two primary particles with signs s, $-s$ and momenta $\mathbf{n}' = \mathbf{n}+\mathbf{l}$, $\mathbf{n}' = \mathbf{n}-\mathbf{l}$, and continues its free flight evolution until a given time T. The created pair, in turn, generates new pairs, etc., and the number of particles increases exponentially. By noting that particles are indistinguishable and that two particles in the same spatial cell with the same momentum $\mathbf{m}$ and opposite signs do not contribute to the Wigner distribution function, an annihilation technique can be implemented to reduce the number of particles during the simulation.[13] The time-dependent evolution of the Wigner quasi-distribution happens only by creation and annihilation of particles which replace the acceleration due to Newtonian forces.[13]

III. NUMERICAL EXPERIMENTS

We study the effects of random processes on quantum systems and the appearance of decoherence in terms of time irreversibility. Indeed, coherence and time reversibility are completely equivalent concepts.[11] Another convenient, and equivalent, criterium is the purity of a system.[15] This quantity can be defined in several ways. For example, it can be expressed in terms of a Wigner quasi-distribution function, of a density matrix, or even of a wave function $\Psi = \Psi(\mathbf{x})$ for the evolution of only pure states

$$p(t) = \sum_{\mathbf{m}=-\infty}^{+\infty} \int_{\mathbf{0}}^{\mathbf{L}} d\mathbf{x} f_W^2(\mathbf{x}, \mathbf{m}, t), \quad (9)$$

$$= Tr(\rho^2) = \int_{\mathbf{0}}^{\mathbf{L}} d\mathbf{x}\rho^2(\mathbf{x}, \mathbf{x}), \quad (10)$$

$$= \int_{\mathbf{0}}^{\mathbf{L}} d\mathbf{x} \int_{\mathbf{0}}^{\mathbf{L}} d\mathbf{x}' \Psi(\mathbf{x})\Psi^*(\mathbf{x}')\Psi(\mathbf{x}')\Psi^*(\mathbf{x}). \quad (11)$$

A convenient physical interpretation can be given, when $p(t)$ is expressed by means of a density matrix. As long as the system evolves in a superposition of pure states, the purity is constant and equal to one. Indeed, the non-diagonal elements are all equal to zero. When, instead, the system enters a decoherent regime, the purity decreases (mixed states).[18]

The initial conditions for the performed experiments consist of a Gaussian wave packet, with minimal uncertainty, interacting with a potential wall represented by a truncated step function whose edge defines the interface of the system. The corresponding initial pseudo-distribution function reads

$$f_W^0(\mathbf{x}, \mathbf{m}) = Ne^{-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{\sigma^2}} e^{-(\mathbf{m}\Delta\mathbf{k}-\mathbf{k}_0)^2\sigma^2}, \quad (12)$$

where N, $\mathbf{k}_0$, $\mathbf{x}_0$, and σ are, respectively, a constant of normalization, the initial wave vector, the initial position, and the width of the wave packet. Its initial position is close to the barrier in order to see the interactions happening at early times. The initial wave vector is chosen such that it corresponds to an energy in equilibrium with the lattice (about 0.025 eV) and has a diagonal component which goes towards the interface. The wall has an energy equal to 0.05 eV, σ is equal to 10 nm. Finally, open BCs which absorb particles, when they reach the edges of the spatial domain, are imposed. In this context, one expects two kinds of processes to happen, partial reflection from the interface and absorption of the packet through the boundaries.

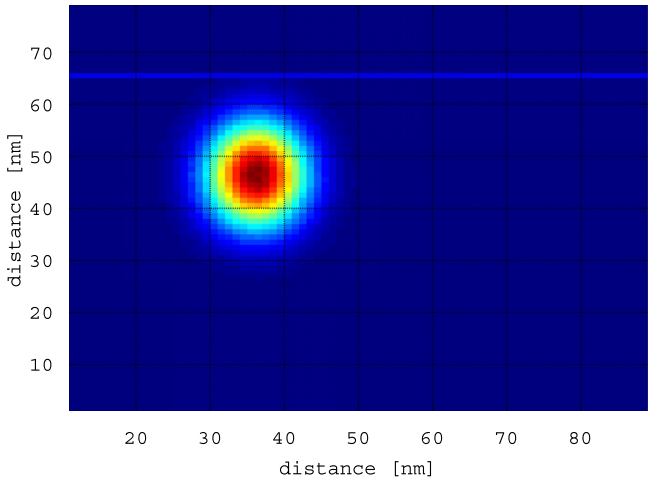

FIG. 1. Forward evolution of a wave packet in proximity of a barrier step at 0 fs.

This system is simulated in five different situations: (1) a flat interface with specular reflection, (2) a rough interface with specular reflection, and a flat interface in the presence of (3) constant inelasticity, (4) random inelasticity, and (5) a diffusive process. All simulations proceed forward in time until 40 fs, when the wave vectors of all particles are reverted in sign. Then the simulation proceeds until 80 fs. This is equivalent to proceed backward in time until 0 fs. The solutions obtained are compared to the initial conditions. To enhance the statistical analysis and reduce the noise, we perform an average over four different instances of the same simulation started with different random seeds.

Finally, Figs. 4, 6 and 8–10 are obtained by cutting in the middle of the normalized wave packet in the y-direction.

A. Time-reversibility

We simulate a wave packet moving towards a flat interface without inelastic or diffusive processes. The goal of this experiment is to show that the Wigner MC method based on particle's signs is suitable for the study of decoherent phenomena. Figs. 1–3 show the results of the simulation. In

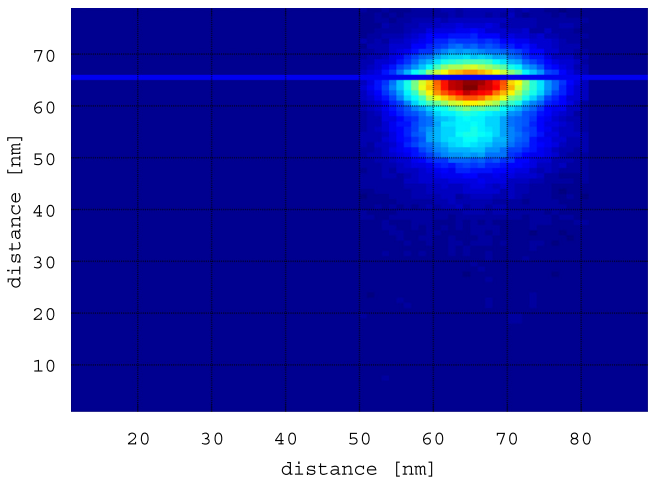

FIG. 2. Forward evolution of a wave packet in proximity of a barrier step at 40 fs. The particles momenta are reverted and the evolution becomes backward in time.

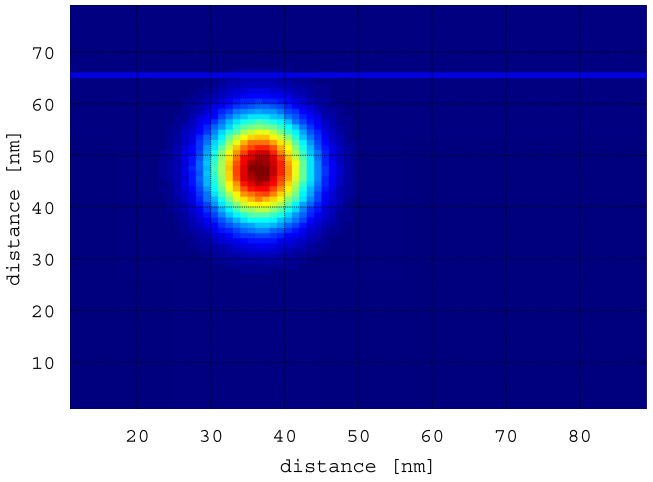

FIG. 3. Backward evolution of a wave packet in proximity of a barrier step at 80 fs.

particular, Fig.1 represents the initial wave packet in proximity of the interface (upper straight line); the bottom plot shows the evolution of the packet at 40 fs, when the wave vectors of all particles are reversed. Finally, the reconstructed solution is reported in Fig. 3. The comparison between the initial solution and the reconstructed solution is reported in Fig. 4. The agreement is excellent. As expected, the system is numerically time reversible and no decoherence is observed.

B. Roughness

We now introduce roughness and mimic a technologically realistic situation. Our methodology consists of adding a position dependent random offset to an initially flat interface. In practice, we start from a set of points representing the flat interface, (x_n, W), where $W = 65$ nm, $n = 1 \ldots N_x$, and N_x is the total number of cells in the x-direction. Then we generate N_x random numbers r_n (uniformly distributed between 0 and 1) and calculate the N_x offsets $\Delta W_n = A(2r_n - 1)$, with A the biggest allowed offset. The interface roughness is now represented by the set of points $(x_n, W + \Delta W_n)$, see Fig. 5 (wavy upper line). Figs. 5 and 6 report the results of the simulation.

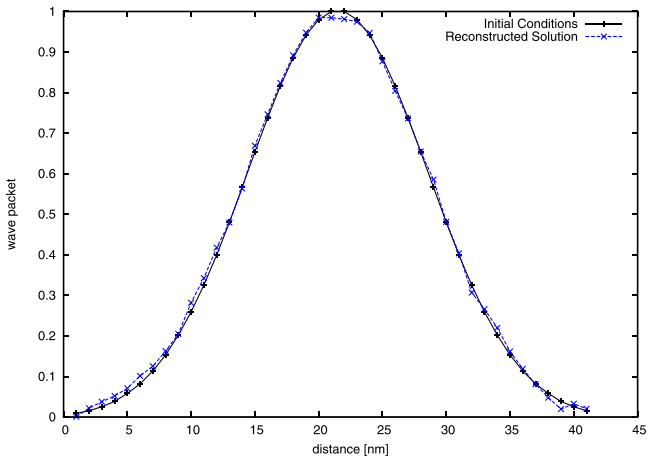

FIG. 4. Comparison (cut in the x-direction) between the initial conditions and the backward solution at 80 fs.

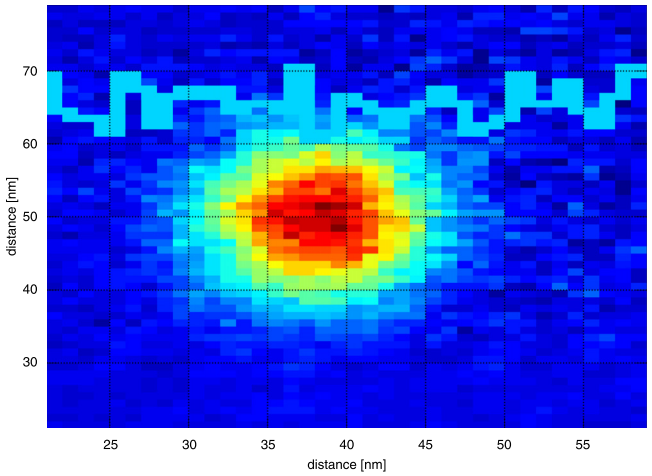

FIG. 5. Forward evolution of a wave packet in proximity of a rough wall at 20 fs.

Fig. 5 shows how important is the shape of the interface in the evolution of the wave packet. Indeed the wave packet is influenced almost instantaneously and rapidly destroyed (some level of chaos is introduced). Nevertheless, the system remains in a coherent state as shown in Fig. 6 (comparison between the initial solution and the reconstructed one). Despite the presence of roughness, the initial state is perfectly reconstructed. A further confirmation that the system is still time-reversible comes from the calculation of the purity. Indeed the (red) + curve of Fig. 7 shows that it remains constant until the wave packet starts to move out of the domain (at about 128 fs).

C. Constant inelasticity

We now introduce an inelastic process in the simulation. Every time a particle reaches the interface, a constant amount of energy is removed from the k_y-component of its wave vector $\mathbf{k} = (k_x, k_y)$ and it is scattered back by inverting its sign. The component k_x is not changed. The amount of energy is chosen arbitrarily and equal to $32\Delta k_y$ with $\Delta k_y = \frac{\pi}{L_C^y}$. Intuitively, the bigger the energy removed, the bigger is the influence of the interface on the system. The

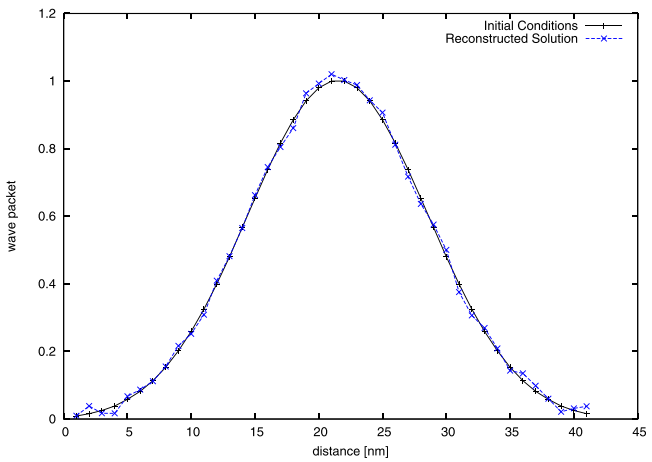

FIG. 6. Comparison (cut in the x-direction) between the initial conditions and the backward solution at 80 fs.

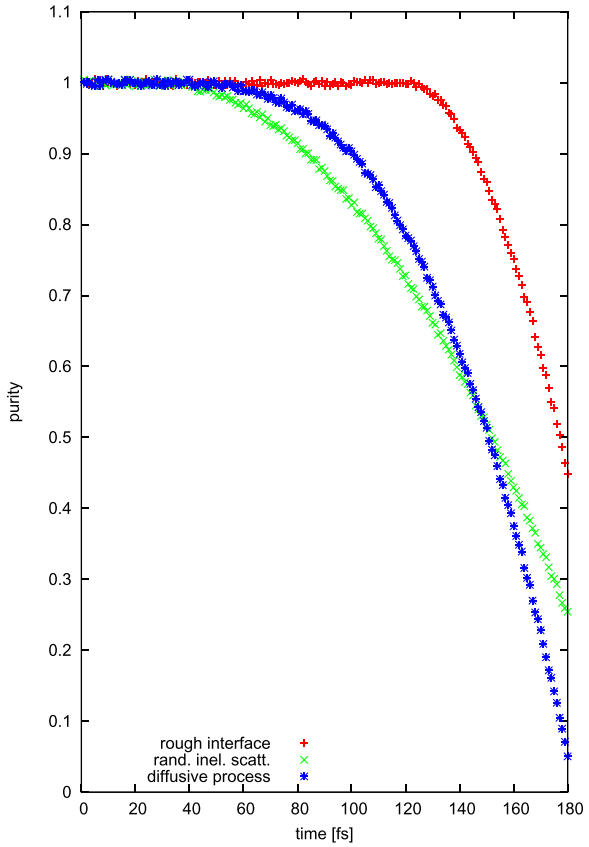

FIG. 7. Purity curves calculated for several numerical experiments. The purity is initially constant and starts to decrease, when the particles interact with a random process (when present) or with the open BCs. The quantum information is lost at a regular pace. The purity of the diffusive process decreases faster than the one corresponding to the random inelastic process. Note that this tendency depends on the particular values used to simulate those processes and, as such, can be inverted.

comparison between the initial and reconstructed solutions is reported in Fig. 8. A big hump of particles is now accumulating in proximity of the wall (right side of the plot) in the reconstructed solution. In other words, the constant inelastic process introduces decoherence, part of the quantum

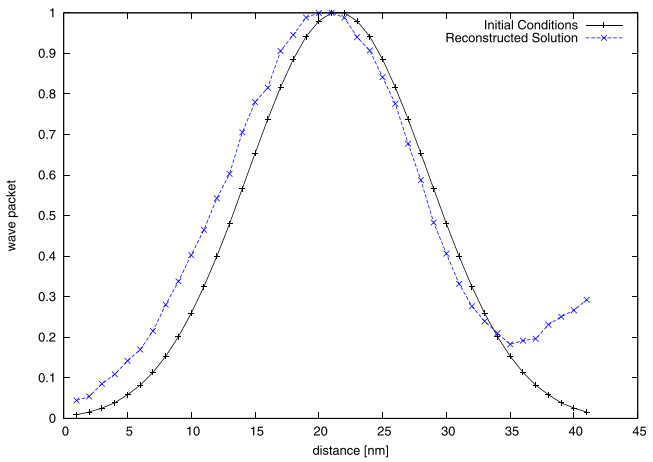

FIG. 8. Comparison between the initial conditions and final backward solutions (at 80 fs) in the presence of constant inelasticity. Note that the cuts are performed after the wave packets are normalized on the two-dimensional domain.

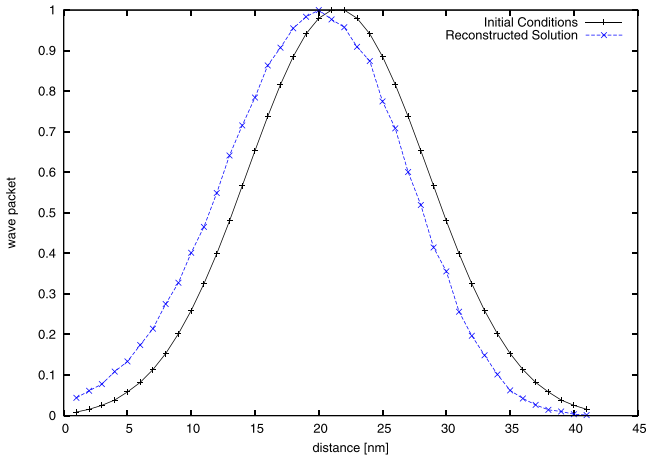

FIG. 9. Comparison between the initial conditions and final backward solutions (at 80 fs) in the presence of random inelasticity.

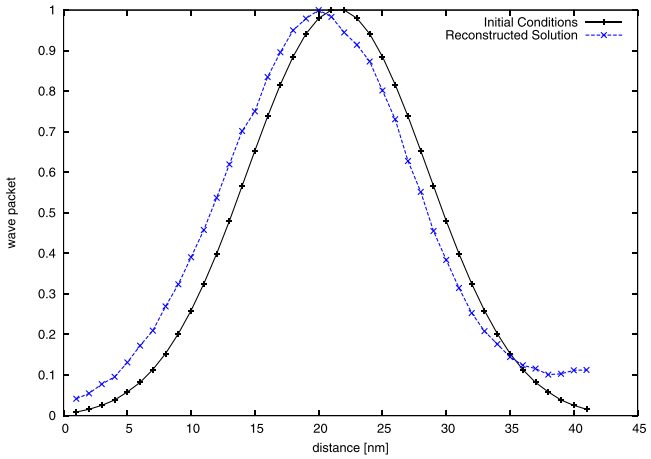

FIG. 10. Comparison between the initial conditions and final backward solutions (at 80 fs) in the presence of a diffusive process.

information is lost, and it is not possible to recover the initial conditions anymore.

One detail must be underlined here: in this experiment, when the system is evolved backward in time the interface keeps on absorbing energy. It can be shown numerically that if, during the backward evolution, the interface adds the same amount of energy (known a priori) to a particle (instead of subtracting it), the initial conditions can be reconstructed. In other words, a constant inelastic process can be inverted and the initial conditions can be reconstructed.

D. Random inelasticity

A random inelastic process is now introduced at a flat interface. In this model, a particle reaching the interface is back scattered and a random amount of energy is subtracted to its k_y component. The quantity is randomly chosen between 0 and $64\Delta k_y$. The comparison is reported in Fig. 9. The system is clearly not time reversible any longer.

One should also note that the comment made in the previous experiment on the reconstruction of the initial conditions by inverting the behavior of the interface during the backward evolution does not hold anymore. Indeed, if the inelastic process is intrinsically random, it cannot be inverted. As soon as a particle interacts with the interface, the information of the system is lost. This is also confirmed by the (green) x curve of Fig. 7 showing the purity of such a system.

E. Diffusive process

We introduce a diffusive process at a flat interface. The wave vector of a particle interacting with the interface is randomly modified in direction, but its energy is kept constant, which corresponds clearly to an elastic process. This can be considered as a generalization of the previous experiment, which is diffusive but also inelastic. The results of the simulation are reported in Fig. 10. The system is not time reversible. Despite its apparent simplicity, this is an important result with profound implications. It shows that inelasticity is not the only process that can trigger decoherence. A confirmation of this fact comes from the calculation of the purity (blue * curve of Fig. 7), which decreases as soon as particles start to be randomized in direction. In other words, the appearance of decoherence is intimately connected to the process of randomization which is the first cause of time irreversibility. It gradually destroys the information and makes it impossible to recover the initial conditions.

F. Conclusions

In this work, we performed a study of the appearance of decoherence at the nanometer scale by applying the Wigner MC method based on particle's signs. The criterium utilized for this investigation is time reversibility. When only a flat interface is involved and no diffusive or inelastic processes are present, the system is time reversible. We have shown that, even when the interface has some level of roughness, time reversibility still holds. When an inelastic process is introduced (by removing a constant or random amount of energy to the particles), the system becomes time irreversible. Then we noted that, when the inelasticity is constant, it is possible to invert the behavior of the interface and make the system time reversible again. This fact does not hold for a random inelastic process which is, by definition, intrinsically stochastic. Finally, we simulated the presence of a diffusive process which randomizes the wave vector of the particles interacting with the interface. This model can be considered a generalization of random inelasticity. From the calculation of the purity, it is clear that the system looses information and becomes time irreversible. This shows that a pure randomization process is enough to make decoherence appear. In other words, randomness is the first cause of time irreversibility.

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[1]R. Rosati, F. Dolcini, R. C. Iotti, and F. Rossi, Phys. Rev. B **88**, 035401 (2013).
[2]B. Vacchini and K. Hornberger, Eur. Phys. J. Spec. Top. **151**, 59–72 (2007).
[3]J. J. Halliwell, J. Phys. A, Math. Theor. **40**, 3067–3080 (2007).
[4]P. Schwaha, D. Querlioz, P. Dollfus, J. Saint-Martin, M. Nedjalkov, and S. Selberherr, J. Comput. Electron. **12**, 388–396 (2013).
[5]D. Querlioz, J. Saint-Martin, and P. Dollfus, J. Comput. Electron. **9**, 224–231 (2010).
[6]P. Schwaha, M. Nedjalkov, S. Selberherr, and I. Dimov, in *LSSC Conference Proceeding* (Springer, 2011), pp. 472–479.
[7]N. Kluksdahl, W. Potz, U. Ravaioli, and D. K. Ferry, Superlattices Microstruct. **3**, 41–45 (1987).
[8]W. Frensley, Phys. Rev. B **36**, 1570 (1987).
[9]K.-Y. Kim and B. Lee, Solid-State Electron. **43**, 2243–2245 (1999).
[10]L. Shifren and D. K. Ferry, Phys. Lett. A **285**, 217–221 (2001).
[11]D. Querlioz and P. Dollfus, *The Wigner Monte Carlo Method for Nanoelectronic Devices—A Particle Description of Quantum Transport and Decoherence* (ISTE-Wiley, 2010).
[12]M. Nedjalkov, H. Kosina, S. Selberherr, Ch. Ringhofer, and D. K. Ferry, Phys. Rev. B **70**, 115319 (2004).
[13]M. Nedjalkov, P. Schwaha, S. Selberherr, J. M. Sellier, and D. Vasileska, Appl. Phys. Lett. **102**, 163113 (2013).
[14]J. M. Sellier, www.nano-archimedes.com.
[15]P. Schwaha, M. Nedjalkov, S. Selberherr, and I. Dimov, in *LSSC 2011, LNCS* (Springer-Verlag, 2012), Vol. 7116, pp. 472–479.
[16]E. Wigner, Phys. Rev. **40**, 749 (1932).
[17]G. Manfredi and M. R. Feix, Phys. Rev. E **62**, 4665 (2000).
[18]U. Fano, Rev. Mod. Phys. **29**, 74–93 (1957).