Phonon-Induced Decoherence in Electron Evolution

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Abstract. A Monte Carlo analysis of the evolution of an electron interacting with phonons is presented in terms of a Wigner function. The initial electron state is constructed by a superposition of two wave packets and a pronounced interference term. The results show that phonons effectively destroy the interference term. The initial coherence in wave vector distribution is pushed towards the equilibrium distribution. Phonons hinder the natural spread of the density with time and advance it towards a classical localization. The decoherence effect due to phonons, which brings about the transition from a quantum to a classical state, is demonstrated by the purity of the state, which decreases from its initial value of 1, with a rate depending on the lattice temperature.

1 Introduction

Quantum computational and communication processes rely on the fundamental physical notions of superposition, entanglement, uncertainty, and interference. The idea for such processes is related to the fundamental physical limits of computation, which are foreseeable due to the saturation in down-scaling the feature sizes of transistors, the basic elements of today's computing engines. Today, features are already characterized by the nanometre scale, where few tens of atom layers represent the active region of devices. As the physical laws at such scale are inherently quantum mechanical in nature, the idea for quantum computations arises in a natural way. The research on quantum computing is mainly concerned with the possible speed-up, quantum complexity bounds, and construction of optimal quantum algorithms [1].

The foundations for quantum algorithms rest on the basic quantum units of information (qubits) and the basic logical manipulations provided by quantum gates. The qubit is a quantum state which may be conveniently presented by the states 0 or 1 of the classical bit forming the basis $|0\rangle$ $|1\rangle$. Any normalized superposition

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad (1)$$

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of such states is a legitimate qubit. A single classical register can store the states only one at a time, while the quantum counterpart stores superpositions of them. In general, a quantum computer with n qubits can be in an arbitrary superposition of up to 2^n different states simultaneously, whereas a normal computer can only be in one of these 2^n states at any given time. The difficult task, however, is to retrieve this information efficiently. The complex numbers α and β can only be measured statistically, which is related to the very nature of quantum mechanics as will be seen below. The property (1) also gives rise to quantum teleportation, since the states can be highly non-local, and to quantum cryptography. In quantum communication it is easy to detect, if the state has been subject to undesired observation, since measurements disturb quantum states, due to the entanglement of $|\psi\rangle$ with the states of the detector. The realizations of all these novel and fascinating scientific ideas rely on the condition that (1) remains coherent, i.e. is a subject of unitary evolution, which is equivalent to say 'remains quantum', since measurements and processes of interaction with the environment try to turn the quantum system into a classical one, a process known as decoherence. To clarify the difference we recall that expectation values $\langle A\rangle$ of physical quantities A, presented by a Hermitian operator $\hat{A}$ are obtained by the trace operation:

$$\langle A\rangle = Tr(\hat{A}\hat{\rho}) = \sum_{i=0,1} \langle i|\hat{A}\hat{\rho}|i\rangle; \qquad Tr(\hat{\rho}) = 1. \tag{2}$$

The density operator $\hat{\rho}$ is defined with the help of (1):

$$\hat{\rho} = |\psi\rangle\langle\psi| = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1| + \alpha\beta^*|0\rangle\langle 1| + \alpha^*\beta|1\rangle\langle 0| \tag{3}$$

The physical quantity 'expectation value for the first basis state' in (1), for example, expressed by the operator $\hat{\rho}_0 = |0\rangle\langle 0|$, evaluates to $|\alpha|^2$ using the trace operation, while for the second state it yields $|\beta|^2$. The relation $|\alpha|^2 + |\beta|^2 = 1$ allows to interpret these values as probabilities, which implies the normalization of (1) and ensures the last equality in (2).

In order to measure quantities we need to prepare a detector which discriminates states $|0\rangle$ from $|1\rangle$ by virtue of their orthogonality. There are two peculiarities of this process. The measurement disturbs the superposition state (1) by leaving it in the measured state. The probability of finding the system in the alternative state after the measurement is zero. Moreover, the last two terms in (3) remain unobservable for such a detector. However, they can be observed by other kind of detectors and actually reveal the quantum character (1): they account for the superposition of the amplitudes which lead to interference effects.

If these interference effects are neglected, the density operator $\hat{\rho}$ reduces to $\hat{\rho}_{\text{cl}} = |\alpha|^2\hat{\rho}_0 + |\beta|^2\hat{\rho}_1$. This density operator again provides the values $|\alpha|^2$ and $|\beta|^2$ for the basis states, however, it corresponds to an entirely different set-up of the system. The latter measures the register by generating *either* the state 0 with a probability $|\alpha|^2$, *or* the complementary state with the complementary

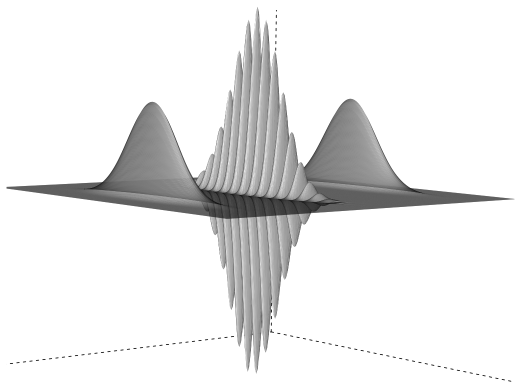

Fig. 1. Entangled wave packets used as initial condition

probability. The collapse of (1) into one of the two possible basis states as a result of a measurement gives rise to the same $\hat{\rho}_{\mathrm{cl}}$, which is a return to the principles of the classical computer. Accordingly, $\hat{\rho}_{\mathrm{cl}}$ can be called classical density operator.

Decoherence destroys the unitary evolution of the coherent state and is thus the biggest enemy of an effective practical realization of the aforementioned ideas. The system interacts with the environment so that system and environment states entangle into a common, usually macroscopic state. The system state now is obtained by applying a trace on the additional variables, which precludes certain correlations. The theory of decoherence addresses the manner in which some quantum systems become classical due to such entanglement with the environment. The latter monitors certain observables in the system, destroying coherence between the states corresponding to their eigenvalues. Only preferred states survive consecutive 'measurements' by the environment as in the above example. The remainder of states which actually comprises a major part of the Hilbert space is eliminated. Many of the features of classicality are actually induced in quantum systems by their environment [2]. The role of scattering has been intensively studied by different models describing quantum Brownian motion. Peculiar for the equation governing the evolution of the density matrix in the spatial coordinate representation $\langle x|\hat{\rho}|x'\rangle$ is a term giving rise to an exponential damping in time with a rate Λ of the off-diagonal elements $(x \neq x')$. Thus the initial wave packet of an electron does not follow the natural process of spreading due to the coherent evolution, but shrinks around the line $x = x'$ revealing a classical localization [3].

Recently the problem has been reformulated in phase space giving rise to a Wigner equation with a Fokker-Planck term describing the diffusion in the phase space [4]. The analysis of the equation provides an alternative interpretation of the process of decoherence in phase space. Quantum coherence effects as a rule give rise to rapid oscillations of the Wigner function. The diffusion

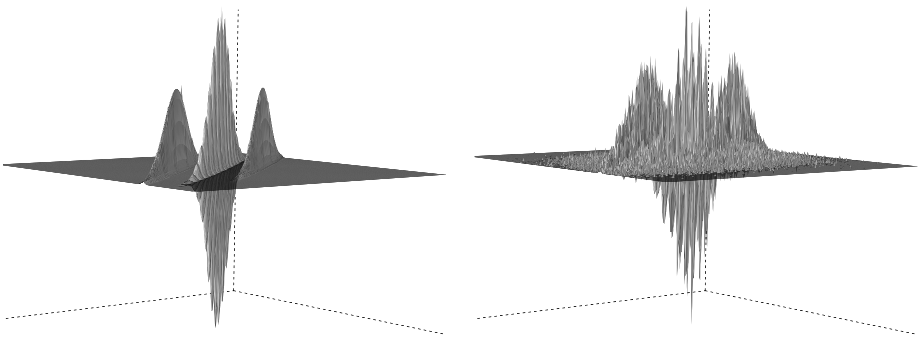

Fig. 2. Left: The coherent evolution leaves the basic structure of the entangled wave packets intact even after 900fs. Right: Scattering mechanisms destroy the initial structure of the Wigner-function as shown here after 300fs.

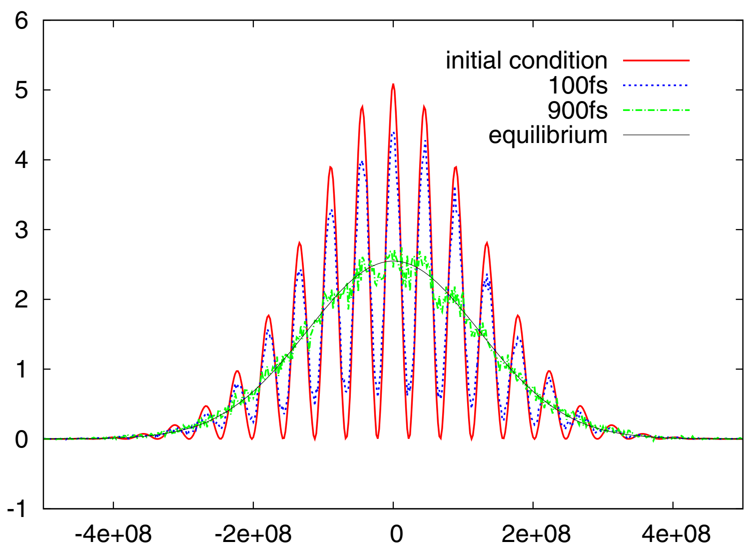

Fig. 3. The momentum distribution of the initial condition decays to at a temperature $T = 200K$ the thermal equilibrium in approximately 1ps. Without scattering the initial distribution remains frozen in place.

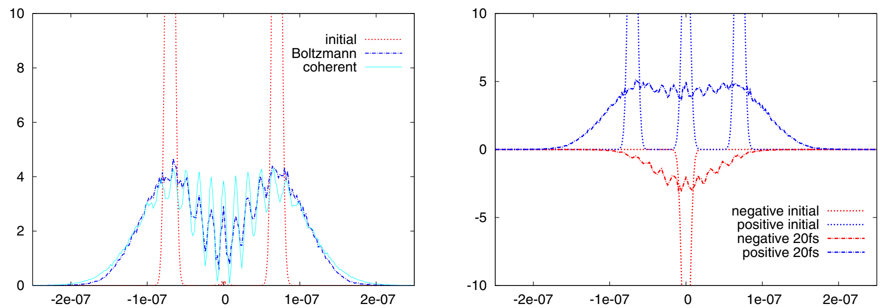

Fig. 4. Left: Initial, coherent and Boltzmann evolution after 200fs at 200K. Right: Positive and negative contributions to the density.

term destroys these oscillations thus effectively suppressing quantum coherence effects. Furthermore, this model has been compared with the Wigner-Boltzmann equation showing that the latter reduces to the former provided that the wave vector of the lattice vibrations becomes much smaller than the electron counterpart [4]. It follows that decoherence effects can definitely be expected as a result of the scattering by phonons. These effects have been well demonstrated by Monte Carlo simulations of the evolution of a single wave packet [4].

We utilize Monte Carlo simulations for analysis of the decoherence caused by the phonon scattering on the evolution of the Wigner function of two wave packets which initially superimpose into a state in the form of (1). We employ a standard weighted Monte Carlo approach which cannot be discussed further due to space constraints. The main indicator is the purity of the state, which decreases from its initial value of 1, with a speed depending on the lattice temperature. The Wigner-Boltzmann model is introduced in the next section. Simulation results and their analysis via a comparison with the coherent evolution are presented in the last section. The results show that phonons effectively destroy the interference term. The initial coherence in wave vector distribution is pushed towards the equilibrium distribution. Phonons hinder the natural spread of the density with time and advance the system towards a classical localization.

2 Wigner-Boltzmann Equation

The Wigner picture provides a unitary equivalent to the rigorous density matrix description of quantum mechanics, and can account for interaction with phonons via the following evolution equation:

$$\left(\frac{\partial}{\partial t} + \frac{\hbar k_{\mathrm{x}}}{m}\frac{\partial}{\partial x}\right) f_{\mathrm{w}}(x, \mathbf{k}, t) = \int dk_{\mathrm{x}}{}' V_{\mathrm{w}}(x, k_{\mathrm{x}}{}' - k_{\mathrm{x}}) f_{\mathrm{w}}(x, k_{\mathrm{x}}', \mathbf{k}_{\mathrm{yz}}, t) \\ + \int d\mathbf{k}' f_{\mathrm{w}}(x, \mathbf{k}', t) S(\mathbf{k}', \mathbf{k}) - f_{\mathrm{w}}(x, \mathbf{k}, t)\lambda(\mathbf{k}) \quad (4)$$

Here, the phase space is formed by a single position and three wave vector coordinates. Quantum correlations are described by the arguments x and k_x of the Wigner potential V_w. Phase-breaking processes are accounted for by the Boltzmann scattering operator with $S(\mathbf{k}, \mathbf{k}')$, the scattering rate for a transition from $\mathbf{k}$ to $\mathbf{k}'$. $\lambda(\mathbf{k}) = \int d\mathbf{k}' S(\mathbf{k}.\mathbf{k}')$ is the total out-scattering rate. The Wigner function f_w is a real quantity. Physical averages are obtained according to $\langle A \rangle = \int d\mathbf{k} dx A(x, \mathbf{k}) f_w$, where A is a generic dynamical function in phase space. Thus, f_w resembles the classical distribution function. However, in contrast to the latter, it allows negative values. Actually, the only positive Wigner function is the equilibrium Maxwell-Boltzmann distribution f_{MB}. Moreover, this is the only function which equates the two terms in the scattering operator and thus remains unchanged by scattering.

In the following, we consider the case without electric potential, so that the V_w term disappears. At first glance (4) reduces to the classical field less Boltzmann equation in this particular case. This, however, is not true, since the classification of the equation depends on the initial condition. If it is non-negative and normalized to unity, this is indeed a legitimate classical distribution function. Alternatively, a phase space function f_w^0 may be chosen, which corresponds to a fully coherent initial system. In this case the uncertainty relation is manifested by the shape of the function: the shape is such that the density matrix $\langle x|\hat{\rho}|x'\rangle$ obtained from the function must be a product of the type $\psi(x)\psi(x')$ where ψ is a quantum state function [5]. Then equation (4) describes the evolution of f_w^0 due to processes of scattering. In the next section we demonstrate that this evolution transforms f_w^0 towards a classical distribution by destroying all incorporated coherence effects.

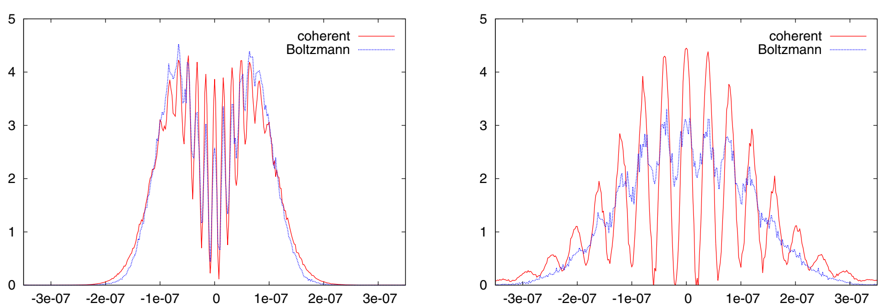

Fig. 5. The spatial broadening of the wave packet is hindered by scattering processes. The coherent wave packet is slightly broader after 200fs (left hand side); with this trend continuing so that the coherent wave packet begins to reach beyond the simulation domain after 500fs, while the wave packet experiencing scattering still exists completely within the confines of the simulation.

3 Simulations and Analysis

The chosen initial condition is the superposition (1) of two Gaussian wave packages: $e^{\frac{-(x\pm a)^2}{2\sigma^2}} e^{\imath bx}$. The corresponding initial Wigner function

$$f^0_{\mathrm{w}}(x,k_{\mathrm{x}}) = N\mathrm{e}^{-(k_{\mathrm{x}}-b)^2\sigma^2}\left[\mathrm{e}^{-\frac{(x-a)^2}{\sigma^2}} + \mathrm{e}^{-\frac{(x+a)^2}{\sigma^2}} + \mathrm{e}^{-\frac{x^2}{\sigma^2}}\cos\left((k_{\mathrm{x}}-b)2a\right)\right] \quad (5)$$

comprised by two Wigner wave packets and oscillatory term is shown in Figure 1. Equilibrium is assumed in the other two directions of the wave space, so that $\frac{\hbar^2}{2\pi m kT}\mathrm{e}^{-\frac{\hbar^2(k'^2_{\mathrm{y}}+k'^2_{\mathrm{z}})}{2mkT}}$ multiplies (5) to give $f^0_{\mathrm{w}}(x,\mathbf{k})$. A GaAs semiconductor with a single Γ valley and scattering mechanisms given by elastic acoustic phonons and inelastic polar optical phonons is considered, while setting the parameter $a = 70$nm. The choice of $2\sigma^2 = \frac{\hbar^2}{2mkT}$ along with $b = 0$ gives rise to $f_{\mathrm{MB}}(\mathbf{k})$, which minimizes the effect of the phonons on the change in the shape of the wave vector distribution. The SI units [m], [m^{-1}] and [s] are used.

During a coherent evolution the initial structure of the Wigner function remains intact, as shown in the left hand side of Figure 2. The oscillatory term corresponding to the off-diagonal elements of the density matrix is responsible for the coherence of the state, since the **k** distributions of the other two components (in k_{y} and k_{z}) remain unchanged. Thus the oscillatory term is most affected by scattering as seen on the right hand side of Figure 2. Indeed, the shape of the initial momentum distribution, $f(k_{\mathrm{x}}) = \int dx dk_{\mathrm{y}} dk_{\mathrm{z}} f_{\mathrm{w}}$, in Figure 3 is due entirely to the oscillatory term, as the other two components of **k** are distributed according to thermal equilibrium, which is indicated by the thin line. The initial shape remains frozen during coherent evolution, while as it is deducible from the figure, scattering destroys the coherence in about $1ps$ and forces the distribution to equilibrium.

Figure 4 shows the density $n(x) = \int dk_{\mathrm{x}} dk_{\mathrm{y}} dk_{\mathrm{z}} f_{\mathrm{w}}$. The coherent curve exhibits pronounced oscillations, which are being suppressed in the Boltzmann curve which localizes around the initial peaks. The initially well balanced positive and negative contributions of f_{w} to the density are destroyed by scattering, as seen on the right hand side of Figure 4. Another effect is that scattering tries to reduce the spreading of the wave packets as can be observed in Figure 5. These results show that scattering induces a spatial localization and destroys coherence, thus preventing reversibility in time. A measure for this behaviour is the purity $p = \int dx dk_{\mathrm{x}} dk_{\mathrm{y}} dk_{\mathrm{z}} f^2_{\mathrm{w}}$. For coherent evolution it remains 1 while the loss of information in the initial state is given by its decrease. An increase of the temperature leads to increase of the electron-phonon coupling and thus an accelerated drop of purity, as depicted in Figure 6.

It is concluded that phonons are an important cause of decoherence. The transition from a quantum to a classical electron state occurs at a picosecond time scale, which acts as a limit for the speed of operation of future semiconductor quantum computers.

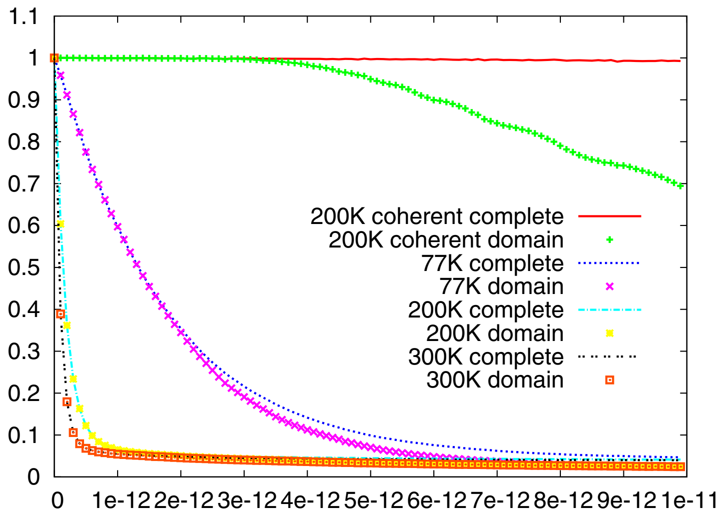

Fig. 6. Evolution of purity at different temperatures. Pairs of lines are obtained by neglecting particles which leave the simulation domain (domain) and by a complete record of all particles (complete). The former case may lead to an artificial indication for loss of coherence.

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