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Analysis of lense-governed Wigner signed particle quantum dynamics

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We present a Wigner signed particles analysis of the lense-governed electron state dynamics based on the quantitative theory of coherence reformulated in phase space terms. Electrostatic lenses are used for manipulating electron evolution and are therefore attractive for applications in novel engineering disciplines like entangletronics. The signed particle model of Wigner evolution enables physically intuitive insights into the processes maintaining coherence. Both, coherent processes and scattering-caused transitions to classical dynamics are unified by a scattering-aware particle model of the lense-controlled state evolution. Our approach bridges the fairly new theory of coherence with the Wigner signed particle method.

1 Introduction The refraction of an electron state on the surface between two domains with different potentials V_1 and V_2 is described by a notion equivalent to Snell's law: $\mathbf{k}_1 \sin\theta_1 = \mathbf{k}_2 \sin\theta_2$ or $\sin\theta_2 \sin\theta_1 = \epsilon\mathbf{k}_1/\epsilon\mathbf{k}_2$, where x is along and y normal to the interface, $|\mathbf{k}|$ is the wave vector length, and θ is the angle between the wave vector and the y-direction. These simple relations give rise to an approach for electron state control, where specially shaped potentials (acting as lenses) are used to focus, guide, reshape, or split an electron state into components. In particular, the electron state can be decomposed by the lense into well established density peaks which may be directed to propagate in desired directions. Of importance are scenarios where the evolution process retains initial coherence which, however, is destroyed by decoherence processes like scattering with lattice vibrations, that is phonons. The electron dynamics, being a complicated interplay between such processes, can be conveniently analyzed in phase space using the Wigner theory [1].

Quantum coherence is the underlying concept of quantum information disciplines and for emerging quantum engineering disciplines such as entangletronics. It is thus surprising that the rigorous theory for quantification of coherence has been suggested only recently [2]. The developed theory follows the ideas of the corresponding quantification theory of entanglement. Moreover, it has been demonstrated that the two concepts are quantitatively equivalent [3], that is, any nonzero amount of coherence in a system can be converted into an equal amount of entanglement between that system and another initially incoherent one [4]. This means that the two concepts which describe very different physical notions have a common mathematical foundation. The mathematical approach has been developed in the framework of operator mechanics, in terms of Hilbert spaces, eigenbasis sets, and tensor products. The formal quantification of coherence in terms of the information theory is based on identifying a set of states $\mathcal{I}$ with the label "incoherent" and a class of incoherent operations which map $\mathcal{I}$ onto $\mathcal{I}$.

The first goal of our work is to show that the Wigner formalism provides a legitimate theoretical framework which presents the basic notions of the quantification theory of coherence in phase space terms. Furthermore, the resulting criteria for coherence in phase space in conjunction with a Wigner signed particle method [5] are applied to analyze a splitting mechanism by the lense electron dynamics. The main results reveal (i) how the splitted parts interact with each-other to maintain the coherence; (ii) how phonons break this interaction, striving to impose classical evolution; and (iii) how incoherent states – defined by the novel theory of coherence – are incorporated in this picture. The analysis is supported by scattering-aware Wigner simulations of the splitting process.

In the next section, we show that the basic notions from the quantitative theory of coherence can be presented in phase space by the Weyl–Wigner map.

2 Coherence in phase space terms In the following, operators are denoted by the "hat" symbol $\hat{()}$, while the indices i, j label the eigenstates of the chosen basis. For simplicity, in this section we consider a one-dimensional phase space x, p.

The Weyl map $A(x,p) = W(\hat{A})$:

$$W(\hat{A}) = \int \frac{\mathrm{d}s\mathrm{d}q}{h} \mathrm{Tr}\left(\hat{A} e^{\frac{i}{\hbar}(s\hat{x}+q\hat{p})}\right) e^{-\frac{i}{\hbar}(sx+qp)} \tag{1}$$

defines an isomorphism from the algebra of operators $\hat{A}(\hat{x},\hat{p})$ with a product and a commutator [,] to the algebra of phase space functions $A(x,p)$ with a non-commutative star (*)-product and a Moyal bracket $[,]_M$ given by:

$$A*B = \mathscr{W}\left(\hat{A}\cdot\hat{B}\right); \quad i\hbar[A,B]_M = \mathscr{W}\left(\left[\hat{A},\hat{B}\right]\right). \tag{2}$$

We introduce the nondiagonal eigenvector Wigner function $f_{ij}(x,p)$ for the eigenvectors $|a_i\rangle$ of the operator $\hat{A}$ of a given physical observable. The following correspondences characterize the map:

$$|a_i\rangle\langle a_j| \leftrightarrow f_{ij}(x,p) = \frac{1}{h}\mathscr{W}(|a_i\rangle\langle a_j|) \tag{3a}$$

$$\hat{A}|a_i\rangle = a_i|a_i\rangle \leftrightarrow (A*f_{ii})(x,p) = a_i f_{ii}(x,p) \tag{3b}$$

$$\hat{\rho} = \sum_\beta P_\beta |\psi_\beta\rangle\langle\psi_\beta| \leftrightarrow f_w(x,p) = \frac{1}{h}\mathscr{W}(\hat{\rho}) \tag{3c}$$

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \frac{1}{i\hbar}\left[\hat{H},\hat{\rho}\right] \leftrightarrow \frac{\mathrm{d}f_w}{\mathrm{d}t} = \frac{1}{i\hbar}[H,f_w]_M \tag{3d}$$

$$\langle A\rangle = \mathrm{Tr}\left(\hat{\rho}\hat{A}\right) \leftrightarrow \langle A\rangle = \int (f_w A)(x,p)\mathrm{d}x\mathrm{d}p. \tag{3e}$$

In the case of $A = H(x,p)$, Eqs. (3a) and (3b) involve states and energies of the Hamiltonian function H.

$\beta \in B$ (cf. Eq. (3c)) labels the pure states $\hat{\rho}_\beta = |\psi_\beta\rangle\langle\psi_\beta|$ with probabilities P_β, so that the Wigner function f_w can be expressed as a linear combination of pure state Wigner functions $f_w^\beta(x,p) = \frac{1}{h}\mathscr{W}(|\psi_\beta\rangle\langle\psi_\beta|)$ or via the nondiagonal functions f_{ij}. The second equation shown in (3d), is the Wigner equation. The relation in Eq. (3e) allows to use the classical expressions $A(x,p)$ for the physical observables.

The equation system (3a)–(3e) demonstrates the full algebraic equivalence of the operator and Wigner formalisms. Any operator mechanics results obtained by algebraic considerations can be expressed in Wigner terms and vice-versa.

The Weyl map allows to transfer the concepts of the information theory of coherence in the Wigner phase space picture. In particular, the definition of coherence becomes: For a fixed basis $|a_i\rangle$ one has to use Eq. (3a) for the set of eigenvector Wigner functions f_{ij} to define the incoherent states as

$$\hat{\sigma} = \sum_i P_i|a_i\rangle\langle a_i| \leftrightarrow f_{w,\sigma} = \sum_i P_i f_{ii} \tag{4}$$

where P_i are probabilities. The set of such states is denoted by $\mathcal{I}$. Any other state which cannot be written in this way is defined coherent [4]. Incoherent states involve only diagonal elements f_{ii}. From Eq. (3a) we conclude that coherence is directly related to the existence of nondiagonal elements f_{ij} in the state representation of f_w.

Finally the measure for coherence in phase space $C(f_w) = \min\mathscr{D}(f_w, f_{w,\sigma})$ where $f_{w,\sigma} \in \mathcal{I}$ is introduced from the measure for distance $\mathscr{D}$. The latter can be based on the von Neumann entropy or trace distance [2]. We note that the time evolution of the linearized von Neumann entropy, or purity, has been already used for the analysis of the reduction of coherence and time reversibility due to random interfaces [6].

In this way, the rules and notions of the resource theory of coherence have been reformulated in terms of phase space functions, establishing the Wigner formalism as a legitimate approach for analysis of coherent processes.

3 Wigner signed particles In the following, we summarize the concepts of signed particles, needed for our analysis. First derived from the Wigner formalism [5], these concepts can be postulated to derive back the Wigner theory [7]. Thus the signed particle approach is fully equivalent to the Wigner formalism[1]. Furthermore, it enables considerable physical insights into various quantum mechanical processes. The signed particle approach: (i) point-like particles with classical features, such as drift over Newtonian (field-less) trajectories and of Boltzmann type scattering carry the quantum information by their positive or negative sign [8]; (ii) physical averages $\langle A\rangle$, Eq. (3e), in a phase space region are given by the sum $\sum_n \mathrm{sign}(n)A_n$ for all particles n in this region; (iii) couples of one positive and one negative particles are generated by rules dictated from (3d) and propagate in space by distinct but fixed momentum which may be changed only by a scattering event; (iv) particles with opposite sign which meet in the phase space annihilate each-other. The annihilation property is crucial for understanding how scattering strives to impose classical, incoherent behavior.

[1] This is in full analogy with the Boltzmann particle model which can be used to derive the Boltzmann equation, but actually contains more physical information, since the Boltzmann particle model describes also processes of noise and correlation.

In the next section, the developed phase space notions and the signed particle model are applied to analyze lense-governed scattering-aware quantum dynamics.

4 Lense-governed quantum dynamics The concept of electrostatic lenses was experimentally first demonstrated in 1990 accompanied by computer simulations [9, 10]. Coherent effects of focusing and splitting of a single electron state have been investigated by Wigner simulations [11, 12]. We present scattering-aware simulations of lense-controlled electron dynamics. They are used to support the analysis of the roots of coherence in terms of signed particles and validate the intuitive model of the process of decoherence. The simulations have been conducted with ViennaWD [13] in a two-dimensional phase space, denoted by $\mathbf{x} = (x, y)$, and $\mathbf{p} = (p_x, p_y)$.

Figure 1 shows a typical electron splitting experiment, where an initial Wigner pure state (corresponding to a minimum uncertainty wave packet $\Psi_{\rm min}$) moves along the y-direction towards the lense. The initial Gaussian-shaped envelope of plane waves (the chosen basis $e^{i\mathbf{p}_j x/\hbar}$) identifies the nondiagonal Wigner basis as $f_{ij}(\mathbf{x},\mathbf{p}) = e^{ix(\mathbf{p}_i-\mathbf{p}_j)}\delta\Big((\mathbf{p}_i+\mathbf{p}_j)/2 \pm \mathbf{p}\Big)$ which has the ability to form interference patterns. In contrast, incoherent states (cf. Eq. (4)) are represented by $\delta(\mathbf{p}_i \pm \mathbf{p})$ which characterizes a classical particle with fixed momentum and an even distribution in the phase space. Thus classical and incoherent perceptions become synonyms so that a loss of coherence is equivalent to a transition to classical behavior. A major part of the state is already located in the region of the lense potential after 75 fs of evolution. The generation of particle couples takes place according to (iii) and thus negative particles begin to appear. In the process of evolution the newborn particles move according to (i) in all directions of the space, in turn generating couples of new particles. After 150 fs the electron is outside the region of the lense and is split into two symmetric and well separated density peaks (cf. Fig. 2). It is important to note that the two

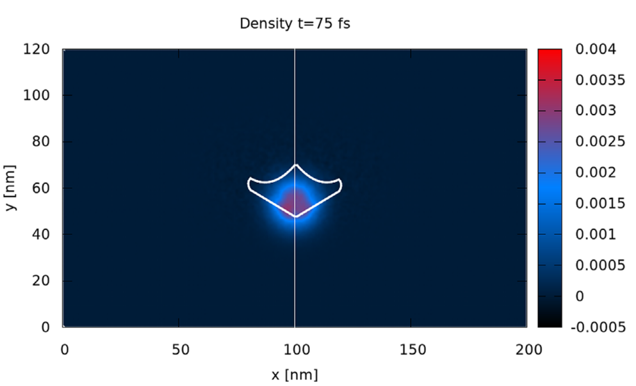

Figure 1 Electron density after 75 fs evolution of the initial minimum uncertainty condition. The white shape shows the electrostatic lense.

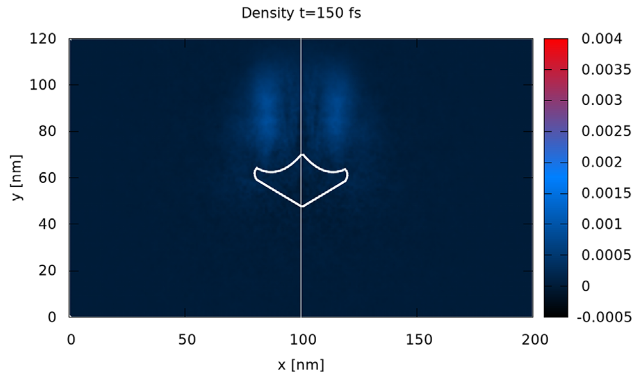

Figure 2 Electron density after 150 fs evolution. Two well established density peaks leave the lense.

peaks cannot be considered as two separated electrons which advance in the phase space in an eventually entangled way. Indeed, the pure state evolution is time reversible so that if one of the peaks is evolved backwards to the time origin, it will become a subset $\psi_{\rm in} \in \Psi_{\rm min}$. However, $\psi_{\rm in}$ is not a physically admissible state, since the uncertainty relations are violated by subsets of the spatial (momentum) variables defining the minimum uncertainty state $\Psi_{\rm min}$.[2] Thus, the task corresponds to a coherent evolution of a single electron. By virtue of (ii) with $A = 1$, the density in a domain $\Delta\mathbf{x}$ around $\mathbf{x}$ at time t is given by the summation of the signs of all particles there. Contributions give the locally generated particles which are still in $\Delta\mathbf{x}$, together with particles initialized in the past, $t' < t$, at different phase space points $\mathbf{x}', \mathbf{p}'$, whose trajectories, determined by $\mathbf{x}', \mathbf{p}', t'$, cross $\Delta\mathbf{x}$ at the time of interest t. We note that domains with negligible physical density but finite density of signed particles also contribute to the dynamics. Furthermore, any changes of the density in the given domain causes corresponding changes in the rest of the space as imposed by the normalization condition.

Any process which influences the free movement of the signed particles not only modifies their distribution and thus the expectation values of the physical quantities (cf. Eq. (3e)), it also reduces the interaction between the phase space regions and thus causes decoherence. The latter is often associated and demonstrated by the emblematic model of quantum Brownian motion, described by the Fokker–Planck equation. Since this equation is obtained as a limit of a more general model, obtained by the inclusion of phonon scattering in the Wigner electron evolution [14], we consider the effect of the phonons on the splitting process. It is important to note that phonons strive to impose equilibrium behavior and that the equilibrium distribution of a quantum electron in a potential belongs to the set of incoherent states (cf. Eq. (4)). Indeed, the Wigner representation of the Gibbs operator is of the form $\sum_\beta P_\beta f_w^\beta$, where P_β are given by the equilibrium distribution

[2] The case that $\psi_{\rm in}$ is proportional to $\Psi_{\rm min}$, is not possible, since the evolution would recover both peaks.

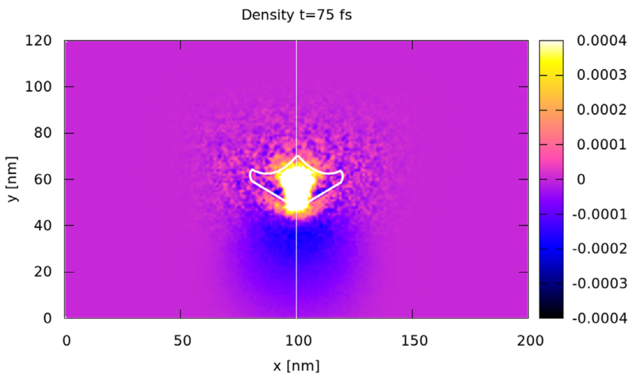

Figure 3 Difference between the coherent densities and those affected by phonons after 75 fs evolution. Phonon scattering mechanisms for silicon are considered, however, the coupling constants have been increased five times, resulting in a five times increase of the scattering frequency, which better illustrates the effect of decoherence.

function of the energy E_β. The latter, together with the eigenstate Wigner functions f_w^β, are given by Eq. (3b). Thus, phonons destroy the coherence, striving to transform the quantum state evolution towards an incoherent state.

The random change of the momentum not only prevents a particle to follow it's coherent behavior impeding the interaction between adjacent regions: Particles which would never meet in the phase space under coherent conditions, now, in accordance with (iv) have a finite probability to annihilate. Annihilation effectively destroys the effect of quantum generation. Furthermore, due to the random choice of the after-scattering direction, generated signed particles stay around the common place of birth, thus giving rise to localization. In this way scattering strives to turn the quantum evolution into a classical diffusive evolution. These processes are well demonstrated in Fig. 3, representing the difference of the coherent and phonon-modified densities. The regions where the latter dominates (the difference is negative) are marked in blue. The chosen example illustrates well the transition from quantum to classical behavior.

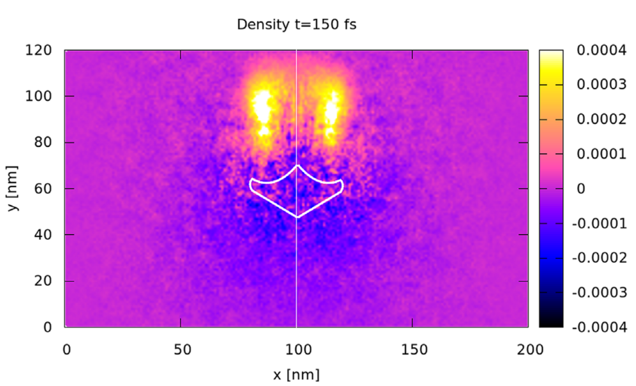

Figure 4 150 fs evolution of the difference between the coherent densities and those affected by phonons. The latter resembles the point-like structure of spreading by scattering induced diffusion of an initial distribution of classical particles.

The quantum initial condition also may be interpreted as an initial classical distribution of electrons. The generated couples of positive and negative particles are annihilated due to scattering, which effectively destroys the quantum effect of the electric potential. Because of the lack of annihilated negative particles, the initial number of positive particles (but not the individual initial particles) remains the same, so that the particle distribution can be described by a classical distribution function. This is pronounced even more after 150 fs of evolution shown in Fig. 4. The spread of the phonon-aware density is restricted as compared to the quantum counterpart, clearly demonstrating the scattering-induced localization.

5 Summary It is shown that the Wigner formalism offers not only a legitimate formulation of the recently developed theory of coherence. The signed particle model of the Wigner evolution, used for analysis of electrostatic lense controlled electron dynamics, provides an intuitive physical picture of the processes which maintain coherence. In particular coherence is associated with the existence of nondiagonal Wigner basis states. In this picture, scattering works against the quantum action of the potential, pushing the evolution towards classical behavior associated with incoherent states.

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