Role of the physical scales on the transport regime

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A relation called scaling theorem is formulated, which estimates how physical scales determine the choice between classical or quantum transport regimes.

The Wigner-Boltzmann equation (WBE) provides a relevant physical model for a variety of transport conditions characterizing modern semiconducting nanostructures [1]. It is defined by two operators, which, as implied by the name, impose quantum-coherent or scattering dominated evolution. While the former is manifested by oscillations in the solution due to quantum superpositions, the second strives towards classical equilibrium causing decoherence and irreversibility. Which of these regimes will prevail, depends on the physical scales whose role is investigated here. The physical system considered is of an electron interacting with a device potential $V(\mathbf{R})$ and a sea of phonons with wave vector $\mathbf{Q}$ and energy $\hbar\omega_{\mathbf{Q}}$ and coupling $\tilde{F}(\mathbf{Q})$ The system is characterized by the scales for length L and energy V_0, which further determine the scales for time $T_0 = \sqrt{\frac{m}{V_0}}L$ and momentum $P_0 = T_oV_o/L$. They are used to express the Hamiltonian in terms of the dimensionless quantities: $\mathbf{R} = L\mathbf{r}$, $\mathbf{Q} = \frac{1}{L}\mathbf{q}$, $V(\mathbf{R}) = \eta V_0 v(\mathbf{r})$, $\hbar\omega_{\mathbf{Q}} = \alpha V_0 \Omega_{\mathbf{q}}$, and $\tilde{F}(\mathbf{Q}) = \beta V_0 F(\mathbf{q})$, defining the strength parameters η, α, β, as well as the dimensionless parameter $\epsilon = \frac{\hbar}{T_o V_0}$ used to obtain a hierarchy of important notions. We first consider the coherent case. (i) The dimensionless Schrödinger equation (SE) is derived, along with an estimate called Egorov's theorem [2]: the mean values corresponding to classical (Poisson bracket) and quantum (commutator) evolution for time t of a given observable differ by $O(\epsilon^2 t)$; (ii) The result can then be generalized for mixed states. A dimensionless Wigner theory, where ϵ replaces $\hbar$ of the standard formulas [3], can be developed. In particular the Wigner function is defined from the density matrix ρ_t:

$$f_w(\mathbf{r},\mathbf{p},t) = \frac{1}{(2\pi\epsilon)^3}\int d\mathbf{r}' e^{-i\mathbf{p}\mathbf{r}'/\epsilon}\rho_t(\mathbf{r}+\frac{\mathbf{r}'}{2},\mathbf{r}-\frac{\mathbf{r}'}{2}); \quad (1)$$

(iii) It is then shown that the Wigner evolution becomes closer to a ballistic Liouville evolution as $|f_w - f_L| < O(\epsilon^2 t)$. These ideas are further pursued to derive a dimensionless WBE in terms of $\epsilon, \eta, \alpha, \beta$:

$$Lf_w = \int d\mathbf{p}'\left(\eta v_w f_w + \beta^2 B f_w\right) \quad (2)$$

v_w is the Wigner potential for (1), and B is the Boltzmann collision operator. Equation (2) yields the scaling theorem: AN INCREASE OF THE ELECTRON -PHONON COUPLING BY A FACTOR β' CAUSES A DECREASE OF THE STRENGTH PARAMETERS AS :

$$\epsilon' = \epsilon/\sqrt{\beta'}, \qquad \eta' = \eta/\beta', \qquad \alpha' = \alpha/\beta'. \quad (3)$$

Thus there are two mechanisms which cause in parallel decoherence of the electron system. The first one could be expected from the linearity of SE: an increase of the phonon coupling is equivalent to a relative decrease of η and α. Very important is the second effect related to the decrease of ϵ. According to (iii) the reduction of this parameter makes the quantum evolution closer to the classical counterpart. The scaling theorem elucidates the heuristic picture of a 'scattering-induced reduction of the coherence length', where electrons 'carry' the information about the electric potential during their free flight. Without scattering the flight lasts forever, so that all spatial points are correlated. Alternatively the distance between the correlated points decreases with the increase of the scattering rates, as they give rise to shorter flights. This is now associated to the decrease of the effect of higher order derivatives of the Wigner potential: in the limit $\epsilon \to 0$ only the local electric field survives. Eqn. (2) shows that the specific way of this reduction is related to the establishment of the delta function from the exponent: the contributions to the integral from regions away from the local $\mathbf{r}$ are canceled due to the rapid oscillations of the exponent there. We add to this an insight about the physical factors affecting the limit. The scaling theorem determines classes of physical problems with equivalent numerical aspects. Processes with very different initial conditions, momenta, electron-phonon coupling, phonon energies, and local evolution time may have equivalent evolution provided that these physical quantities are properly scaled. Numerical experiments illustrate this for $\eta = 0$, $\beta' = 2$.

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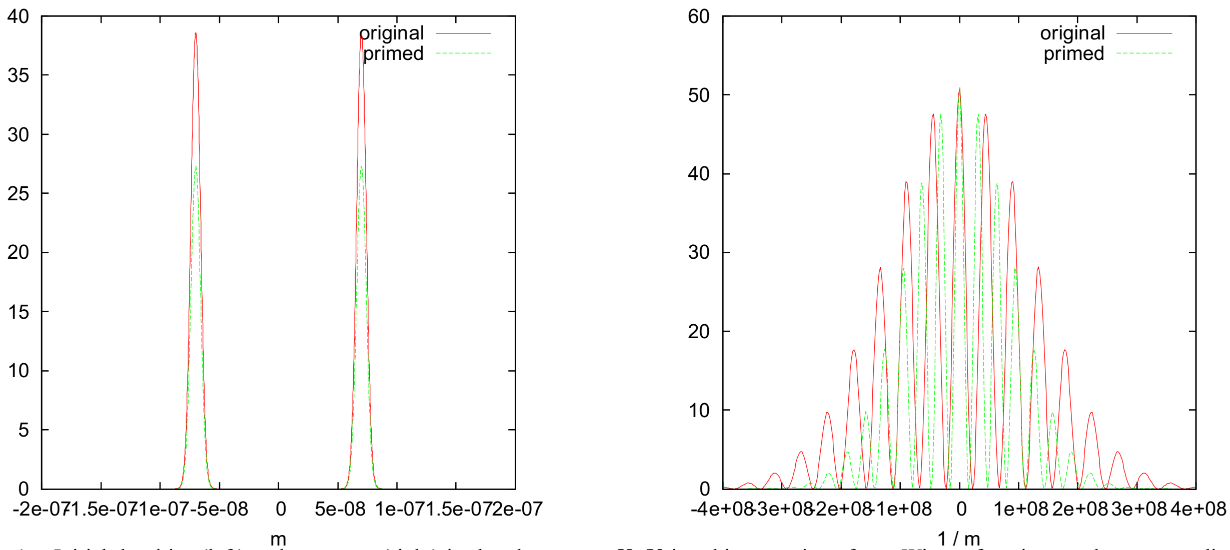

Fig. 1. Initial densities (left) and momenta (right) in the phase space X, K in arbitrary units, of two Wigner functions each corresponding to two entangled Gaussian wave packages. The parameters are scaled as follows: $\epsilon' = \epsilon/\sqrt{\beta'}$, $\alpha' = \alpha/\beta'$, $T_0' = T_0/\sqrt{\beta'}$ and the wave vector scale $K_o' = K_0\sqrt{\beta'}$, where $K_0 = 1/\epsilon L$, in the case of $\beta' = 2$. The two experiments have very different physical characteristics in terms of electron-phonon coupling, phonon energies, and initial distributions $\phi(X, K)$ and $\phi(X', K') = \phi(X, \sqrt{\beta'}K)$. However, according to (3) they correspond to one and the same numerical task.

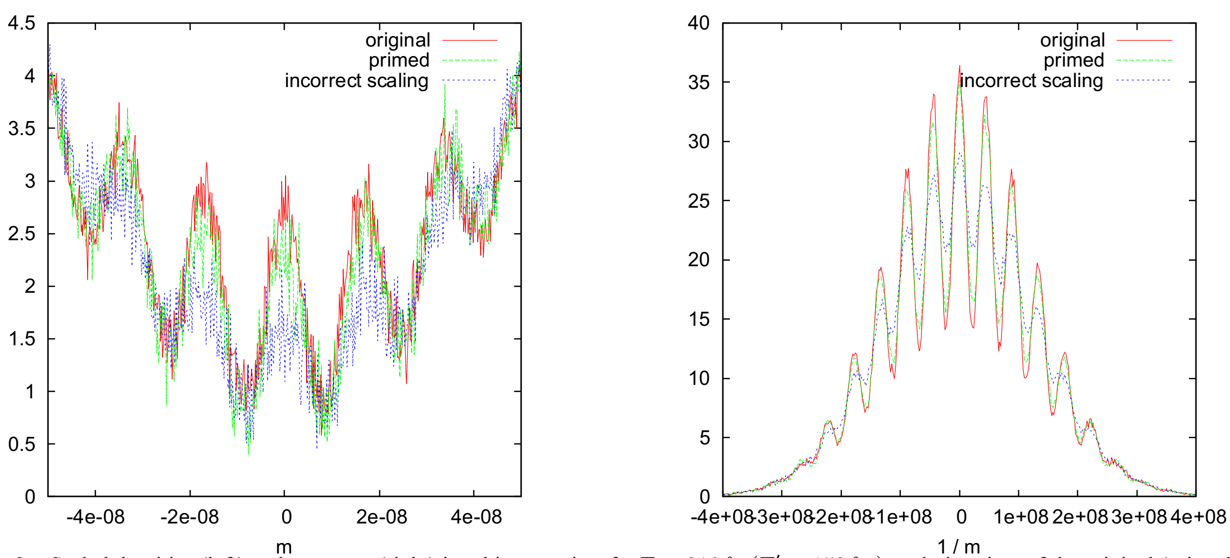

Fig. 2. Scaled densities (left) and momenta (right) in arbitrary units after $T = 210fs$ ($T' \simeq 150fs$.) evolution time of the original (primed) system. The scaled curves fit well within the stochastic noise, showing that they correspond to different stochastic processes, which, however give rise to the same distribution of the mean values. Indeed, a third experiment defined by an inconsistent scaling only of the phonon energy $\alpha' = \alpha/\sqrt{\beta'}$ shows a different behavior. The standard GaAs model with acoustic and optical phonons has been used at a temperature of $200K$.