Role of the Physical Scales on the Transport Regime

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

I. Introduction

The Wigner-Boltzmann (WB) equation 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.

II. Physical Scales

The physical system considered consists of an electron interacting with a semiconductor device potential $V(\mathbf{R})$ and a sea of phonons with wave vector $\mathbf{Q}$ and energy $\hbar\omega_{\mathbf{Q}}$ and coupling $\tilde{F}(\mathbf{Q})$, which define the Hamiltonian of the electron-phonon system:

$$\begin{aligned} H = & - \frac{\hbar^2}{2m}\nabla_{\mathbf{R}} + V(\mathbf{R}) + \sum_{\mathbf{Q}} b^{\dagger}_{\mathbf{Q}} b_{\mathbf{Q}} \hbar\omega_{\mathbf{Q}} \\ & + i\sum_{\mathbf{Q}} \tilde{F}(\mathbf{Q})(b_{\mathbf{Q}} e^{i\mathbf{Q}\hat{\mathbf{R}}} - b^{\dagger}_{\mathbf{Q}} e^{-i\mathbf{Q}\hat{\mathbf{R}}}) \end{aligned} \quad (1)$$

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 $P_0 = T_o V_o / L$. They are used to express the Hamiltonian in terms of the dimensionless quantities:

$$\begin{aligned} &\mathbf{R} = L\mathbf{r}, \quad Q = \frac{1}{L}\mathbf{q}, \quad V(\mathbf{R}) = \eta V_0 v(\mathbf{r}), \\ &\hbar\omega_{\mathbf{Q}} = \alpha V_0 \Omega_{\mathbf{q}}, \quad \tilde{F}(\mathbf{Q}) = \beta V_0 F(\mathbf{q}), \end{aligned} \quad (2)$$

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.

A. Coherent Evolution

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 considered in the phase space. A dimensionless Wigner theory can be developed. The most general formulation of the Wigner function introduces another arbitrary parameter ϵ' as follows:

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

where ρ^{ϵ}_t is the density matrix. The value of ϵ' can be fixed by requesting some properties of the function f_w: it is natural to wish, if possible, to have a function (3) which recovers the classical way of obtaining averages. Calculations show that this is possible, and give rise to the condition $\epsilon' = \epsilon$. In this way a dimensionless Wigner theory may be developed, where ϵ replaces $\hbar$ in the standard formulas [3]. (iii) It is then shown that, if ϵ decreases, the Wigner evolution becomes closer to a ballistic Liouville evolution f_L as $|f_w - f_L| < O(\epsilon^2 t)$.

B. WB Evolution and Scaling Theorem

These ideas are further pursued to derive a dimensionless WB equation in terms of $\epsilon, \eta, \alpha, \beta$:

$$Lf_w = \int d\mathbf{p}' \left(\eta v_w f_w + \beta^2 B f_w\right) \quad (4)$$

where v_w is the Wigner potential corresponding to (3), and B is the Boltzmann collision operator. The following notion, called scaling theorem is formulated.

An increase of the electron-phonon coupling by a factor β' causes a decrease of the strength parameters as:

$$\epsilon' = \epsilon/\sqrt{\beta'}, \qquad \eta' = \eta/\beta', \qquad \alpha' = \alpha/\beta'. \quad (5)$$

III. Effects due to Scattering

A. Effects of Decoherence

The scaling theorem shows that there are two mechanisms which cause in parallel decoherence of the electron system. The first one could be expected from the form of the Hamiltonian (1) and the linearity of the Schrödinger equation: an increase of the phonon coupling is equivalent to a relative decrease of the defined in (2) strength parameters η and α.

The existence of a second mechanism shows that the transition towards classical transport is faster than the transition caused by just a linear decrease of the quantum component. This second mechanism is related to the decrease of ϵ in (5): according to (iii) the reduction of ϵ renders the quantum evolution closer to the classical counterpart. This aspect of the scaling theorem elucidates the heuristic picture of a 'scattering-induced reduction of the coherence length'.

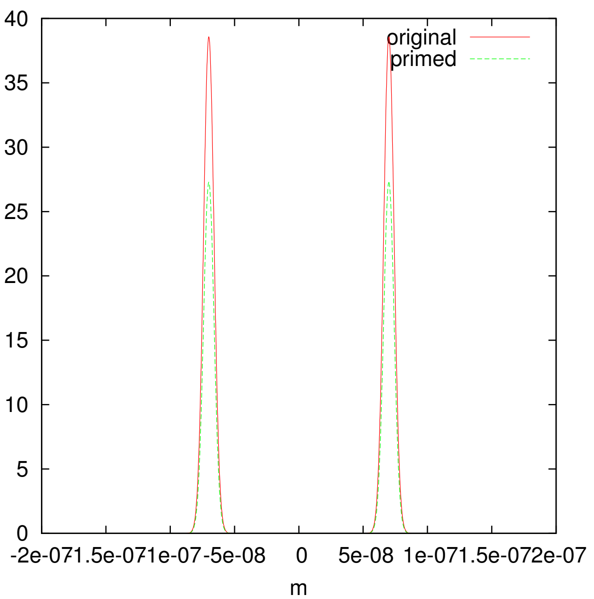

Fig. 1. Initial densities in the phase space X, K of the genuine and primed systems, arbitrary units.

The destructive effect of the scattering on the quantum behavior has been associated with the picture of electrons which 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 model is in the following provided with a mathematical foundation linked 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. An analysis of the Wigner potential term in (4) 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 position $\mathbf{r}$ are canceled due to the rapid oscillations of the exponent when $\epsilon \to 0$. The relationship between the strength parameters adds to this an insight about the physical factors affecting the limit.

B. Evolution Classes

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. The existence of such classes of physically different, but mathematically equivalent problems is demonstrated by considering the evolution of entangled electron states.

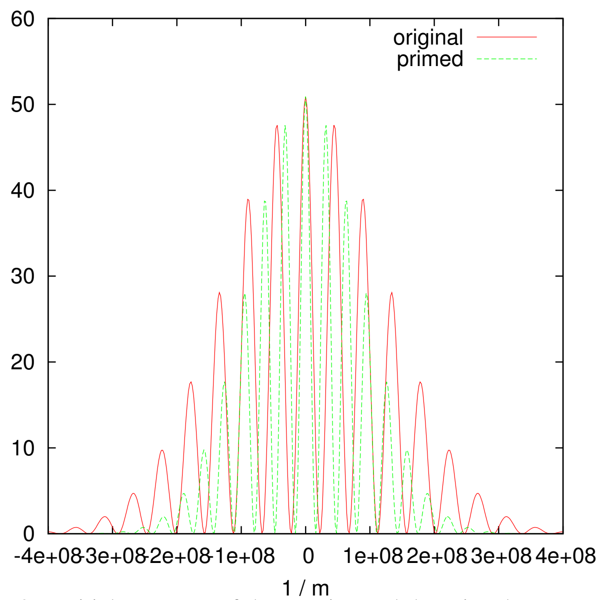

Fig. 2. Initial momenta of the genuine and the primed systems. The third system has the same initial condition as the primed counterpart.

The underlying experiment corresponds to an electron system initialized by superposition of two Gaussian wave packets $e^{-(X\pm X_0)^2/2\sigma^2}e^{iK_0x}$ giving rise to the following initial Wigner function:

$$f_0(X,K_x) = Ne^{-(K_x-K_0)^2\sigma^2}\left(e^{-\frac{(X-X_0)^2}{\sigma^2}} + e^{-\frac{(X+X_0)^2}{\sigma^2}} + e^{-\frac{X^2}{\sigma^2}}cos\left((K_x-K_0)2X_0\right)\right) \quad (6)$$

This initial Wigner function follows a free evolution, where only phonons interact with the electron state. Phonons cause decoherence by effectively destroying the well pronounced oscillatory term on the last line of (6)

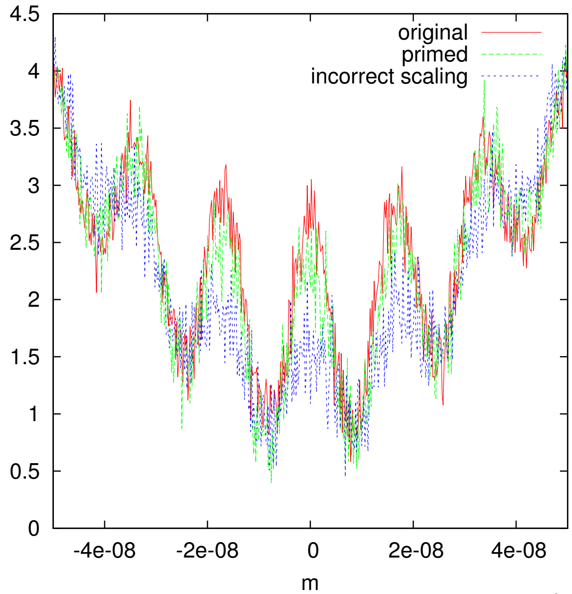

Fig. 3. Scaled densities in arbitrary units after $T = 210fs$ ($T' \simeq 150fs$.) evolution time of the original (primed and third) system.

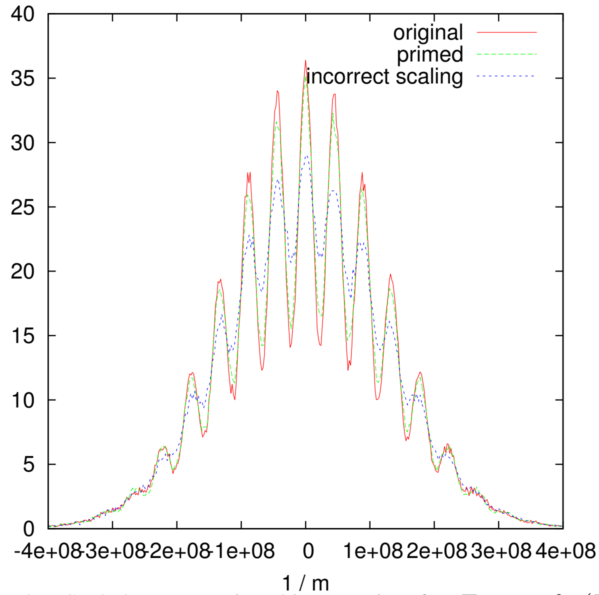

Fig. 4. Scaled momenta in arbitrary units after $T = 210fs$ ($T' \simeq 150fs$.) evolution time of the original (primed and third) system.

during the process of evolution. The initially entangled state evolves towards an object having completely different physical meaning: it is a mixed state, determined by the probabilities of the electron to be in one or the other packets related to the two wave functions. Equilibrium is assumed in the other two directions of the wave space, so that $\frac{\hbar^2}{2\pi mkT}e^{-\frac{\hbar^2(K'^2_y+K'^2_z)}{2mkT}}$ multiplies (6) to give $f_w^0(X,\mathbf{K})$. A GaAs semiconductor with a single Γ valley and scattering mechanisms given by elastic acoustic phonons and inelastic polar optical phonons is considered, $X_0 = 70nm$, the temperature is $200K$. A choice of $2\sigma^2 = \hbar^2/(2mkT)$ along with $K_0 = 0$ gives rise to the Maxwell-Boltzmann distribution, which minimizes the effect of the phonons on the change in the envelope of the wave vector distribution.

Three experiments with different physical settings are carried out The strength parameters of the two of them, called genuine and primed systems are linked by the scaling theorem, while in the third one, only the phonon energy is intentionally modified for comparison. Thus, the third state has the same initial setup as the primed one. The parameters are scaled as follows:

$$\epsilon' = \epsilon/\sqrt{\beta'}, \quad \alpha' = \alpha/\beta', \quad T_0' = T_0/\sqrt{\beta'},$$

and the wave vector scale is

$$K_o' = K_0\sqrt{\beta'}, \quad \text{where} \quad K_0 = 1/\epsilon L.$$

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 $\phi(X',K') = \phi(X,\sqrt{\beta'}K)$. Figure 1 and Figure 2 show the initial distribution of the densities and momenta of the genuine and primed electron states. However, according to (5) they correspond to one and the same numerical task. Figure 3 and Figure 4 show densities and momenta of the three systems after $T = 210fs$ of the genuine system, corresponding to $T' \simeq 150fs$. of the primed one. The scaled curves fit well within the stochastic noise, the latter showing that they correspond to entirely different stochastic processes which give rise to the same distribution of the mean values. The third system, defined by an inconsistent scaling of the phonon energy $\alpha' = \alpha/\sqrt{\beta'}$, shows a different behavior after the same evolution of $150fs$, demosntrating that this system belongs to another evolution class.

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