The $\boldsymbol{R}$-$\boldsymbol{\Sigma}$ Method for Nanoscale-Device Analysis

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***Abstract*— This paper describes part of an investigation that aims at consistently incorporating quantum corrections into the transport model, for applications to advanced solid-state devices. The task is carried out in two steps. The first one derives two equations in which the dynamics of the dispersion of the single-particle wave function is accounted for in addition to that of the expectation value of position. The model is founded on an approximate description of the wave function that eliminates the need of the Ehrenfest approximation. The second step is based on the Lagrangian form of the single-particle equations and incorporates such an extended dynamics into the statistical framework. The theory is suitable for different levels of applications: the first step is applicable to the single-particle ballistic dynamics; the second, after a suitable generalization of the collision terms, to the solution of the Boltzmann equation by the Monte Carlo or other methods, and to the solution of the continuity equations in the position-dispersion space. The paper shows the formalism of the single-particle dynamics and provides some examples of its application to typical test cases, along with comparisons with the corresponding solutions of the Schrödinger equation. The derivation of the balance equations for the collective transport is discussed as well.**

I. Introduction

In a recent paper, a theory has been proposed that leads to a set of two Newton-like equations describing the single-particle dynamics. The dynamical variables of the equations are the expectation value $\boldsymbol{r}$ of the wave function and its dispersion $\boldsymbol{\sigma}$ [1].[1] The equations inherently account for the Heinsenberg position-momentum uncertainty relation and exhibit a term proportional to $\hbar^2$, with $\hbar$ the reduced Planck constant.
The theory has been devised for application to the modeling of advanced solid-state devices, where it is necessary to account for the finite extension of the particles' wave functions. The latter, in fact, plays a non-negligible role due to the device size and to the presence of sharp variations in the electric potential. The key point in the derivation of the set of Newton equations is an approximate method to calculate the average of the force over the wave function. The method allows one to dispose of the Ehrenfest approximation without the need of completely determining the wave function itself. The outcome of the method is the set of equations

$$m\frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = -\frac{\partial V}{\partial x_i} - \frac{1}{2}\sum_{n=1}^{3}\frac{\partial^3 V}{\partial x_i \partial x_n^2}\,\sigma_n\ , \tag{1}$$

[1] At the time of preparing this manuscript the issue and page numbers of references [1] and [2] were not known yet.

$$m\frac{\mathrm{d}^2 \sigma_i}{\mathrm{d}t^2} = \frac{\hbar^2}{2m}\,\frac{1}{\sigma_i} - \frac{\partial^2 V}{\partial x_i^2}\,\sigma_i\ , \tag{2}$$

where $V(\boldsymbol{r})$ is the potential energy, with $\boldsymbol{r} \equiv (x_1, x_2, x_3)$, and m the particle mass. More specifically it is assumed that the particle energies are sufficiently low to make the effective-mass approximation applicable. As a consequence, m is in fact the particle effective mass. Although the tensor nature of it could be included in the calculation, it is not considered here for the sake of simplicity.
In turn, x_i is the ith component of the expectation value of the particle's position and σ_i the ith component of the dispersion of the particle's position. These quantities are given by

$$x_i = \langle \xi_i \rangle = \int |\psi|^2\,\xi_i\,\mathrm{d}^3\xi\ , \tag{3}$$

$$\sigma_i = \int |\psi|^2\,(\xi_i - x_i)^2\,\mathrm{d}^3\xi = $$

$$= \int |\psi|^2\,(\xi_i^2 - x_i^2)\,\mathrm{d}^3\xi > 0\ , \tag{4}$$

with $i = 1, 2, 3$. In (3,4) $\psi(\boldsymbol{\xi}, t)$ indicates the particle's wave function, which is assumed normalized. The integrals are carried out over the domain of ψ.
Eqs. (1,2) describe the dynamics of the expectation value and dispersion of the wave function for a given potential energy V. They provide an improved picture with respect to that given by the expectation value alone, namely,

$$m\frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = -\frac{\partial V}{\partial x_i}\ , \tag{5}$$

which is derived in a straightforward manner by calculating from the standard quantum-mechanical procedure the time derivatives of the expectation values of position and momentum, and by applying the Ehrenfest approximation to the result. In particular, (1,2) incorporate a description of the wave function's dispersion, which is a typical quantum feature because it is related to the non-zero extension of the wave packet. Thus, it is of interest to compare the results derived from (1,2) with those obtained from the solution of the full Schrödinger equation. Such a comparison is carried out in this paper for a number of cases of practical interest.
Having in mind the application of the model to the description of carrier transport in solid-state devices, it is worth pointing out that in the case of a semiconductor crystal the potential

energy V of (1,2) derives only from the perturbations due to the application of an external field and/or the presence of a position-dependent dopant concentration. The effects of collisions are not included in (1,2) and must subsequently be introduced into the transport equation as shown in [2]. It follows that the investigation about the validity range of (1,2) must focus on the short time between collisions in the typical operating regime of solid-state devices.

A qualitative picture about how (1,2) are derived may be given as follows. The physical domain where the particle motion occurs is assumed to be sufficiently small to make the size of the particle's wave function significant. The periodic potential energy due to the crystal is accounted for through the equivalent Hamiltonian. Taking the low-energy case, the latter is expanded to the second order leading to the effective-mass concept. Starting from some initial condition the envelope wave function propagates under the influence of the external field, until a collision occurs or the particle leaves the domain of interest. During the flight the expectation value of the particle position evolves in time, while the wave function undergoes a deformation that makes its dispersion to evolve as well.

From the mathematical viewpoint the expectation value of position is the first-order moment of $|\psi|^2$. The zero-order moment is also present in the theory due to the normalization condition. To improve the description of the particle motion beyond that provided by the expectation value of position, which constitutes the Ehrenfest approximation, it is sensible to take the second-order moment. This is equivalent to add the dispersion as a new dynamical variable. Then, the first step leading to (1,2) is the standard calculation of the time derivative of an expectation value applied to the operators ξ_i and ξ_i^2. The derivation is completed by assuming that $|\psi|^2$ at the initial time has a Gaussian shape, in order to apply the minimum-uncertainty condition.

The concept of equivalent Hamiltonian does not apply any more if a collision occurs. In this case the particle dynamics must be tackled by a full-quantum calculation. The latter provides the transition probabilities per unit time of the dynamical variables conjugate to $\boldsymbol{r}$, $\boldsymbol{\sigma}$.

It is worth observing that the procedure depicted above lends itself to a systematic refinement. In fact, it is known that a function that possesses the moments of all orders can be reconstructed starting from a series made of the moments themselves. A finite number of moments thus provides a partial reconstruction of the function. The refinement is achieved by adding more moments to the truncated series.

In modern solid-state devices it often happens that the domain size in one or two dimensions is so small as to give rise to subbands. In this case (1,2) must be adjusted to account for the dynamics of a suitable subset of variables. Due to their structure, (1,2) will be termed *position-dispersion equations* or, more shortly, R-Σ *equations* to remind the symbols by which these variables are usually indicated in the literature.

The paper is organized as follows: a brief discussion about the R-Σ equations is carried out in section II. Then, the comparison between the outcome of the R-Σ model and the solution of the Schrödinger equation is carried out in section III for the cases of a free particle, of a particle subject to a linear potential energy, and of the linear harmonic oscillator. Section IV deals with the regional approach, namely, the use of piecewise-polynomial approximations for the external potential energy V, and with the treatment of the discontinuities of some derivatives of V at the boundaries. A qualitative discussion of tunneling is carried out as well. Finally, the application of the R-Σ equation to the collective transport is discussed in section V, while the conclusions are drawn in section VI.

II. The $\boldsymbol{R}$-$\boldsymbol{\Sigma}$ equations

Some qualitative features of (1,2) are discussed below. First, the force at the right hand side of each equation is made of two terms. At the right hand side of (1) the first term depends on $\boldsymbol{r}$ only and is the standard component of the force present at $\boldsymbol{r}$ in the Ehrenfest approximation. The second term is a correction that accounts for the wave function's dispersion, and its expression is a mixture of the $\boldsymbol{r}$ and $\boldsymbol{\sigma}$ coordinates. One may notice that the quantity multiplying σ_n in the second term has the dimensions of a pressure. Turning to (2), the first term at the right hand side depends on σ_i only. Also, as σ_i is positive definite, the term $\hbar^2/(2m\,\sigma_i)$ gives rise to a repulsive force that diverges as σ_i approaches zero. Such a force, that prevents σ_i from vanishing, is a consequence of the Heisenberg uncertainty principle inherent in the derivation of the R-Σ equations. The second term at the right hand side of (2) is again a mixture of coordinates. The mixed terms give rise to an exchange of energy between the two sets $\boldsymbol{r}$ and $\boldsymbol{\sigma}$ of degrees of freedom of the particle.

It is interesting to note that the reduced Planck constant $\hbar$ appears only in the first term at the right hand side of (2). Then, it would seem sensible to think of such a term as a quantum correction, that applies to a formally-classical description of the dynamics of a system having six degrees of freedom, and disappears in the classical limit $\hbar \to 0$ leaving behind an equation of motion of the form $m\ddot{\sigma}_i = -\sigma_i\,\partial^2 V/\partial x_i^2$. However this conclusion is not sound, because in the classical limit all the "internal" degrees of freedom σ_i disappear from the equations of motion. Thus it is more correct to consider all internal degrees of freedom as typical of the quantum correction.

It is worth adding a few comments about the fact that, although the original Hamiltonian operator

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla_\xi^2 + V(\boldsymbol{\xi}) \tag{6}$$

is conservative, the R-Σ equations (1,2) deriving from it are not necessarily so, unless some special form is prescribed for the potential energy V. The problem does not occur in the Ehrenfest approximation because the σ_i coordinates are not present there, and the terms involving the x_i coordinates are in gradient form from the very beginning.

The conservativeness of the force field is not essential as long as the description of the particle's dynamics is concerned,

which may be tackled by solving the system of equations (1,2) directly. On the other hand, the Hamiltonian form of the equations provides obvious advantages for both the description of the single-particle dynamics and its extension to the collective-transport case. For this reason, the conservative case only will be considered here, by assuming specific forms of the potential energy V such that the force field of (1,2) is conservative.
More general shapes of V may be described by subdividing the domain of V into small regions and interpolating V in each region by functions that keep the conservativeness of the force field locally. However it must be noted that such a regional approach gives rise to discontinuities in some derivatives at the boundaries between regions. An example of this will be given in section IV. Prior to that, some important cases in which the same form of V holds in the whole $\boldsymbol{r}$ space will be illustrated.

III. EXAMPLES

This section is devoted to the analysis of three important test cases, namely those where the potential energy V is constant, linear, or quadratic. The expectation value x_i and dispersion σ_i provided by the R-Σ equations are compared within a given time range with those derived from the solution of the Schrödinger equation. The analysis of the test cases is important because more complicated shapes of the potential energy may be constructed by a combination of them.
Analysing the dynamics of x_i is straightforward. For instance, when $V = \text{const}$ the dynamics is separated into one-dimensional problems, each associated to a pair x_i, σ_i of degrees of freedom. For x_i the R-Σ equations yield $x_i = x_{i0} + \dot{x}_{i0} t$, where x_{i0}, $\dot{x}_{i0}$ indicate the initial conditions. The result is identical to that obtained from a full-quantum calculation. This is not surprising, as it is known that when the potential energy is constant, linear, or quadratic, the expectation values of position and momentum rigorously satisfy the classical equations of motion (see, e.g., [3, III_D]). For this result to hold it is not necessary to assume any special form of the wave packet at $t = 0$. However, for consistency with the derivation of the R-Σ equations, here and in the following the initial form of the packet is assumed to be Gaussian.
The conclusion is that for a constant, linear, or quadratic potential energy the dynamics of x_i derived from the R-Σ equations (1) is exact at all times.
A more interesting comparison is about the dynamics of dispersion. It is known that the full-quantum calculation of the dispersion of a Gaussian wave packet in free space, valid at all times, provides (see, e.g., Eq. (20) of [3, G_I])

$$\sigma_i = \sigma_{i0} \left(1 + \frac{\hbar^2 t^2}{4\, m^2\, \sigma_{i0}^2} \right) , \tag{7}$$

$\sigma_{i0} = \sigma_i(t = 0)$. The solution of (2) for a free particle is obviously different from (7). However, its first-order expansion in time is exactly equal to (7). As noted before, the comparison is meaningful because the derivation of the R-Σ equations assumes that the wave packet is initially Gaussian as well. However, it is also necessary to check whether the time range where the first-order expansion holds is sensible for the application to the semiconductor-device analysis. The expansion implies the constraint

$$\frac{t^2}{\sigma_{i0}^2} \ll \frac{4m^2}{\hbar^2} . \tag{8}$$

A quantitative estimate may be carried out using the parameters of the conduction band of silicon in the effective-mass approximation. The interatomic distance d_a in the silicon crystal is about 0.233 nm. One may assume that the initial value $\sqrt{\sigma_{i0}}$ of the wave packet's standard deviation along the ith direction is significantly larger than d_a, say, $\sqrt{\sigma_{i0}} = 20\, d_a$. Also, the time interval in which the estimate is to be carried out must be smaller than the average time between collisions τ_c. Considering the case of an undoped crystal subject to a weak electric field, it is $\tau_c \simeq 10^{-13}$ s at room temperature. In the estimate one may use for m the effective mass m_n of the electrons in the conduction band, given by $3/m_n = 1/m_l + 2/m_t$, with $m_l \simeq 0.97\ m_0$ and $m_t \simeq 0.19\ m_0$ the longitudinal and transversal mass at room temperature, respectively, and m_0 the free-electron mass [4]. One finds that for $t < \tau_c$ the approximation is indeed applicable to the problem of interest. For instance, the data used in the graph of Fig. 1 show that at $t = 0.1$ ps the relative error ϵ on the standard deviation with respect to the full-quantum case is about 3.2%. At the relatively large time $t = 0.3$ ps it is still $\epsilon \sim 20\%$.
The approximation is even better if the semiconductor is doped and/or the electric field is high, because such operating conditions make τ_c to decrease.
The discussion above readily extends to the case where the potential energy is a linear function of the coordinates. In fact, as noted before, the dynamics of the expectation value x_i provided by the R-Σ equations is exact at all times for this type of potential energy. As far as the dispersion is concerned, an initially-Gaussian packet spreads in the same manner as in the free-particle case [5]. As a consequence, (7) still holds when the potential energy is linear, and the discussion about the applicability limits of the R-Σ equations to the analysis of semiconductor devices leads to the same conclusions as in the free-particle case.
It is interesting to note that the initial conditions might be prescribed in such a way as to make $\dot{\sigma}_i < 0$ at $t = 0$, so that the dispersion initially tends to decrease with respect to the initial value. However it is easily seen that, when the potential energy V is constant or linear, the term inversely proportional to σ_i at the right hand side of (2) will always make σ_i to eventually increase in time.

Another interesting example is that of a potential energy of the linear harmonic-oscillator type. As in the previous examples the dynamics is separated into one-dimensional problems. Eq. (1) provides an oscillatory motion of x_i around $x_i = 0$ with the same angular frequency ω_i as in the classical case. The full-quantum calculation shows that the expectation value of the wave packet along the ith direction oscillates with the

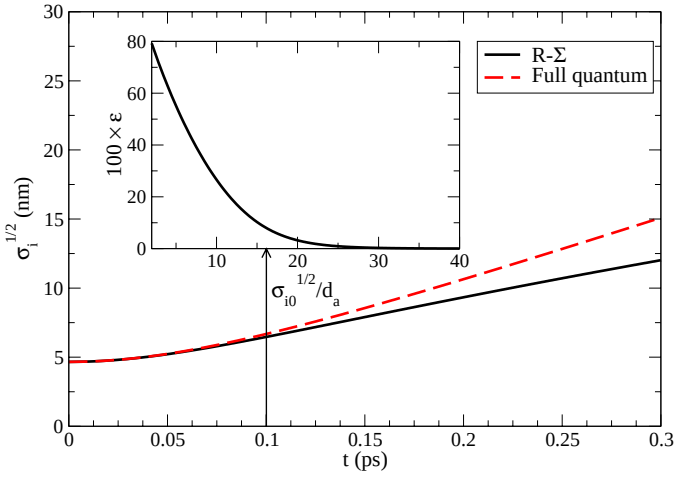

Fig. 1. Comparison of the R-Σ standard deviation $\sqrt{\sigma_i}$ with the full-quantum case as a function of time, for a constant or a linear potential energy. The relative error is defined as $\epsilon \doteq (\sqrt{\sigma_{i\mathrm{FQ}}} - \sqrt{\sigma_{iR\Sigma}})/\sqrt{\sigma_{i\mathrm{FQ}}}$. The inset shows $100 \times \epsilon$ calculated at a fixed time $t = 0.1$ ps for different initial values of the normalized standard deviation. The normalization factor $d_a = 0.233$ nm is the interatomic distance in a silicon crystal at room temperature.

same frequency. This should be expected as already noted at the beginning of this section.

Turning to the dispersion, for a linear harmonic oscillator it is known that in the full-quantum case the dispersion oscillates as well, with an angular frequency $2\omega_i$ (see, e.g., [6, XII]). Again, for this result to hold it is not necessary that the initial packet's form be Gaussian. Correspondingly, the R-Σ equation for the dispersion reads

$$m\,\frac{\mathrm{d}^2\sigma_i}{\mathrm{d}t^2} = \frac{\hbar^2}{2m}\,\frac{1}{\sigma_i} - m\omega_i^2\sigma_i\,, \tag{9}$$

which is seen by inspection to provide an oscillatory motion. In fact, the generalized force that determines the dynamics of σ_i is the sum of two terms. The first one is repulsive from the origin, diverges as σ_i approaches zero, and tends to vanish as σ_i departs from zero. The second one is attractive towards the origin, diverges as σ_i departs from it, and tends to vanish as σ_i approaches zero. These observations are sufficient for concluding that the motion of σ_i is oscillatory. Also, the generalized force has only one zero at $\sigma_{im} = \hbar/(\sqrt{2}\,m\omega_i)$. It follows that the motion occurs in the interval defined by the zeros of

$$\frac{m}{2}\,\omega_i^2\sigma_i^2 - \frac{\hbar^2}{2m}\,\log\frac{\sigma_i}{\sigma_{i0}} = \sigma_{i0}E_{\sigma i}\,, \tag{10}$$

where $E_{\sigma i}$ is the constant energy associated to the degree of freedom described by σ_i. In the actual calculations involving (10) it is convenient to take $\sigma_{i0} = \sigma_{im}$. Note that $E_{\sigma i}$ has no upper limit, whereas its minimum is determined by imposing that the zeros of the left hand side of (10) coincide.

To find whether the R-Σ method catches the oscillation frequency of the dispersion it is necessary to solve (10) numerically. However, its limiting cases can be estimated analytically. One finds that the oscillation frequency tends to the exact limit $2\omega_i$ when $E_{\sigma i}$ increases, whereas it tends to decrease when $E_{\sigma i}$ approaches its minimum. The lower limit of the oscillation frequency is $\sqrt{2}\,\omega_i$. The numerical solution of (10) shows that the estimates are correct, and also that the frequency decrease from $2\omega_i$ to $\sqrt{2}\,\omega_i$ occurs in a very small energy interval near the minimum of $E_{\sigma i}$. Such a behavior is also consistent with the full-quantum calculation.

IV. The regional approach

As anticipated at the end of section II, it is preferable to deal with potential energies that allow for recasting (1,2) in a conservative form, namely, that transform the right hand sides into the components of a gradient. Taking the one-dimensional case by way of example, with coordinates x and σ, it is seen by inspection that the goal is achieved using a piecewise-quadratic form of V. This is similar to the method often used in quantum calculations, where a complicated shape of V is approximated by piecewise-constant functions, and the wave function and its space derivatives are then matched at the regions' boundaries. Here, the matching must be accomplished in time by imposing suitable conditions onto x and σ.

The analysis of the regional approach is easier in the case of (2), which will be illustrated first. Approximating V by a piecewise-quadratic form leads to spatial discontinuities in the second derivative V''. At the time when $x(t)$ reaches a discontinuity point of V'', the acceleration $\ddot{\sigma}$ undergoes a discontinuity in time, while σ and $\dot{\sigma}$ remain continuous. It follows that the constant energy E_σ associated to the degree of freedom described by σ (corresponding to $E_{\sigma i}$ of (10)) may take different values in the intervals between discontinuities.

In parallel, a spatial discontinuity of V'' forces a delta-like behavior of V''' at the same point. This, in turn, induces a time discontinuity of $\dot{x}$, whereas x remains continuous. This makes the energy E_x associated to x discontinuous as well, due to the change in its kinetic part at the discontinuity points. However, it is found that the discontinuities of E_x and E_σ exactly balance each other so that the sum $E_x + E_\sigma$ takes the same constant value over all intervals, as dictated by the conservativeness of the force field. This is an example of the energy exchange between the degrees of freedom that was mentioned in section II.

It is worth adding that the description of the potential energy as a piecewise-quadratic form lends itself to tackling the important cases of particles interacting with steps or barriers. Among these, of paramount importance for modern semiconductor devices is of course the case of tunneling across a barrier. The application of the R-Σ model to the tunneling problem requires a detailed analysis in itself, which is addressed in a separate paper [7]. Here a qualitative-only description will be given, in order to show how the R-Σ equations are indeed able to catch the essence of a non-classical effect such as the tunneling through a barrier.

Still considering a one-dimensional case, let the barrier height be V_M, and let $E_x + E_\sigma$ be the total energy of a particle approaching the barrier. If the energy related to the x degree of freedom equals the barrier height, $E_x = V_M$, the particle's expectation value stops as it reaches the barrier's position, say at $x = 0$. However, the dispersion σ keeps increasing in time, and the standard deviation $\sqrt{\sigma}$ fills up a larger and larger segment of the x axis centered at $x = 0$. Assuming that the particle approached the barrier from the left, the fraction of $\sqrt{\sigma}$ on the left (right) of $x = 0$ may be taken as the reflection (transmission) probability in the frame of the R-Σ model.

If $E_x < V_M$ holds, the expectation value bounces back at $x = 0$. In this case the midpoint of the segment representing the standard deviation is rigidly carried to the left by the expectation value, while the segment's length keeps increasing. Depending on the initial conditions it may happen that the segment's right end lies on the right of the barrier, which corresponds to a non-zero transmission probability. By the same token this description provides a non-zero reflection probability in the case $E_x > V_M$.

It is worth observing that, as far as the expectation value of position is concerned, the possible outcomes of the R-Σ and Schrödinger equations are just the same, although the time dependence of x may be different. This points out that the inclusion of dispersion into the model is essential for providing a description of tunneling, albeit approximate.

V. The collective transport

The R-Σ equations lend themselves to the derivation of a generalized form of the Boltzmann transport equation. This is accomplished by extracting a set of canonically-conjugate dynamical variables from the single-particle equations (1,2) and constructing a Boltzmann-like transport equation by means of the Liouville theorem.

Once the Boltzmann-like equation has been obtained, a set of balance equations for the concentration c of the particles in the $\boldsymbol{r}, \boldsymbol{\sigma}$ space is derived by taking the first-order moments. This is done by multiplying the Boltzmann-like equation by $\dot{x}_i$ or $\dot{\sigma}_i$ and integrating over the space conjugate to $\boldsymbol{r}$, $\boldsymbol{\sigma}$ [2]. As the whole derivation of the balance equations complies with the standard procedure of the transport theory, and remembering that the single-particle equations (1,2) embed a quantum feature through the dispersion, it follows that the R-Σ method provides a sound basis for the inclusion of quantum effects into the equations that describe the collective transport of charge. Thus it constitutes a possible alternative to other methods that have been proposed in the last years, e.g., the *density-gradient correction* [8], [9], in which a correction term is added to the potential energy of the transport model in the $\boldsymbol{r}$ space to obtain an equivalent field acting on the carriers, or the *effective-potential correction* [10], [11], which generalizes the DG correction starting from a convolution of the actual potential energy with the wave function, or the *smooth quantum potential* [12], where an effective stress tensor and energy density for the quantum hydrodynamic equations are derived in the Born approximation to the Bloch equation. It is shown in [13] that the density-gradient correction for a pure state is actually the quantum potential of Bohm [14], which may in turn be traced back to the pilot wave of de Broglie [15], [16]. An interesting analysis about the ability of the density-gradient correction to describe tunneling is carried out in [17].

To complete the collective-transport part it is necessary to incorporate the scattering events into the balance equations. As noted in section I this should be made consistently with the model's formalisms, namely, by parametrizing the wave function by $\boldsymbol{r}$ and $\boldsymbol{\sigma}$. This will be the object of future investigations.

The set of balance equations for the concentration c in the $\boldsymbol{r}, \boldsymbol{\sigma}$ space has a form that lends itself to the application of the standard numerical schemes implemented in commercial simulators. In fact, such a set is made of a continuity equation for c coupled with other equations describing the fluxes in the $\boldsymbol{r}$ and $\boldsymbol{\sigma}$ spaces. Extracting the fluxes and replacing them into the continuity equation yields a scalar, second-order partial-differential equation in the unknown c.

The boundary conditions of the model are standard as well: c is prescribed along some parts of the boundary (typically, the equilibrium distribution may be taken there), while the normal components of the fluxes in the $\boldsymbol{r}$ and $\boldsymbol{\sigma}$ spaces are made to vanish along the remaining parts of the boundary. The equations must eventually be coupled with the Poisson equation that provides the potential energy V as a function of the charge distribution.

VI. Conclusions

The theory depicted in this paper leads, first, to a set of the two R-Σ equations (1,2) describing the expectation value of position and the dispersion of the wave function. The outcome is different from the approaches of [8], [9] and [10], where the quantum-correction term is added to the potential energy of the transport model in the $\boldsymbol{r}$ space, to obtain an "equivalent" field acting on the carriers.

The application to test cases and the comparison with the corresponding solutions of the Schrödinger equation show that the R-Σ equations provide the correct description of the single-particle dynamics within a time range of the order of the average time between collisions in a semiconductor like silicon. This result is encouraging because, next, the model provides the basis for extending the method to the description of the collective transport, following the standard recipe of the transport theory.

Presently a more intensive experimentation is still necessary for the ballistic case, to test the performance of the method in two or three dimensions and to extend its validation to more complicated forms of the potential energy. As anticipated in section IV, this is indeed possible despite the difficulty of finding a Lagrangian form of (1,2) for an arbitrary potential energy V.

As far as the transport aspects of this work are concerned, the model needs to be completed by a consistent calculation of

the scattering terms, followed by a thorough comparison with the approaches of [8], [9], [10], [12].

The derivation of the model based on the R-Σ equations also provides some clues about future refinements of the theory. Remembering the description of section I, the single-particle, ballistic case is improved by considering moments of $|\psi|^2$ of higher orders than the second. As for the transport aspects, the key to future refinements is also apparent in the model proposed here, namely, using higher-order moments of the Boltzmann equation to achieve a set of hydrodynamic-like transport equations following, e.g., the approach of [18], [19]. Finally, as mentioned in section V, the transport equations provided by the R-Σ model are of the same type as those solved by the present commercial simulators. This is a positive aspect in view of the analysis of realistic devices, where the full-quantum approaches may become inapplicable due to the complicate geometries, or too expensive from the numerical viewpoint.

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