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Efficient solution of the Wigner–Liouville equation using a spectral decomposition of the force field

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ABSTRACT

The Wigner–Liouville equation is reformulated using a spectral decomposition of the classical force field instead of the potential energy. The latter is shown to simplify the Wigner–Liouville kernel both conceptually and numerically as the spectral force Wigner–Liouville equation avoids the numerical evaluation of the highly oscillatory Wigner kernel which is nonlocal in both position and momentum. The quantum mechanical evolution is instead governed by a term local in space and non-local in momentum, where the non-locality in momentum has only a limited range. An interpretation of the time evolution in terms of two processes is presented; a classical evolution under the influence of the averaged driving field, and a probability-preserving quantum-mechanical generation and annihilation term. Using the inherent stability and reduced complexity, a direct deterministic numerical implementation using Chebyshev and Fourier pseudo-spectral methods is detailed. For the purpose of illustration, we present results for the time-evolution of a one-dimensional resonant tunneling diode driven out of equilibrium.

1. Introduction

The investigation of electronic transport in electronic devices takes place at a crossroads of computational physics, quantum mechanics and statistical mechanics. With the advent of nanoscaled components, quantum mechanical models replace the older semi-classical models. Nowadays, there are several competing frameworks for calculating the quantum transport models, ranging from simple single particle ballistic wavefunction based methods [1] over the non-equilibrium Green's functions (NEGF) methods [2] to the Pauli master equation [3,4] and the Wigner formalism [5,6].

In the Wigner formalism, one describes a generally mixed quantum state expressed in terms of a Wigner function $f(\mathbf{r}, \mathbf{p}, t)$ living in phase space. Being a quasi-distribution function, the Wigner function acts like a distribution function for the purpose of calculating real observables, but it cannot be used as a real probability function because it can, and does, attain negative values in the presence of quantum mechanical effects [7]. Like the semi-classical Boltzmann transport equation, the Wigner formalism is not limited to calculating the steady state, but can be used to calculate the full time evolution of a state $f(\mathbf{r}, \mathbf{p}, t)$, under the influence of a generally time-dependent potential profile $V(\mathbf{r}, t)$, starting from a given initial state, such as the equilibrium state. Furthermore, technology has progressed to the point that very fast pulsing in the range of picoseconds is available, and already used in the manipulation of charge based quantum well qubits in

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quantum computing [8,9]. The Wigner function formalism is naturally equipped to handle the time-evolution, including mixing of states and decoherence, in these cases.

The quantum mechanical analogue to the classical Boltzmann transport equation, describing the time evolution of the Wigner function is the Wigner–Liouville equation,

$$\frac{\partial}{\partial t} f(\mathbf{r},\mathbf{p},t) + \frac{\mathbf{p}}{m}\cdot\nabla_{\mathbf{r}} f(\mathbf{r},\mathbf{p},t) - \frac{1}{\hbar}\int \mathrm{d}^3p'\, W(\mathbf{r},\mathbf{p}',t) f(\mathbf{r},\mathbf{p}-\mathbf{p}',t) = 0\,, \tag{1}$$

where the Wigner kernel is given by

$$W(\mathbf{r},\mathbf{p},t) = -\frac{\mathrm{i}}{(2\pi\hbar)^3}\int \mathrm{d}^3x\, \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}\left[V\left(\mathbf{r}+\frac{\mathbf{x}}{2},t\right) - V\left(\mathbf{r}-\frac{\mathbf{x}}{2},t\right)\right], \tag{2}$$

where we have omitted the Boltzmann collision integral for the time being. Unlike its classical counterpart, the influence of the potential on the Wigner function through the Wigner kernel is non-local in both position and momentum. This non-locality, combined with the high dimensionality of phase space – typically three times the dimension of the configuration space, makes the Wigner kernel difficult to handle directly.

In literature, we find a range of proposed techniques to tackle this problem. In line with the solution of the Boltzmann equation, there have been significant efforts in solving the Wigner equation using Monte-Carlo, or particle based techniques [6,10–13]. Even though all Monte-Carlo approaches rely on the stochastic solution of the Wigner function, the differences between various Monte-Carlo approaches are significant, from relying on signed particles [10] and Fourier transforms [11] to using spatial decomposition approaches [12,13]. In contrast to the former, the deterministic approaches feature a more direct treatment, which we have adopted in this paper. While having been studied for a long time [14], direct discretization using well-designed finite difference approaches has recently been improved by using the weighted essentially non-oscillating scheme (WENO) to prevent erroneous oscillations [15]. In other work, it has also been shown that the Wigner function can be solved in a robust way using adaptive pseudo-spectral methods in the form of mass-conserving spectral element methods [16,17]. In these methods, the carefully crafted spectral decomposition of the Wigner function enables the oscillatory components introduced by the Wigner kernel to be solved exactly. Finally, the oscillatory quantum effects can also be mitigated by decomposing the potential in a classical and quantum part [18,19].

In this paper, we propose a deterministic method to solve the Wigner equation by exploiting the analogy with the classical Boltzmann transport equation without, however, invoking the classical limit. In contrast to the highly optimized numerical techniques that have been outlined above [6,10–13,15–17], our main focus is on the development of a different, but equivalent form of the Wigner function that allows for a natural, direct implementation. To this end, we recast the Wigner equation into a form that employs the force field rather than the potential energy from which one would conventionally proceed in quantum mechanics. In section 2, we detail the reformulation of the Wigner equations using spectral components of the force field. In section 3 we consider the one-dimensional case and its interpretation based on signed generation terms. In section 4, we describe a one-dimensional numerical implementation of the rewritten Wigner equation using Chebyshev and Fourier pseudo-spectral methods. In section 5, we illustrate our method by tracing the time evolution of electrons propagating through a double-barrier resonant tunneling diode (RTD) driven out of equilibrium. Finally, we conclude in section 6.

2. Using the classical force

Through its appearance in the Wigner kernel, the potential energy $V(\mathbf{r})$ describes the non-local change in momentum of the quasi-distribution function. This is contrasted by the classical counterpart of the Wigner–Liouville equation, the Boltzmann transport equation, where the classical force field $\mathbf{F}(\mathbf{r},t) = -\nabla V(\mathbf{r},t)$ provides a direct, local measure of the change in the momentum coordinate over time. In this section, we recast the quantum mechanical Wigner–Liouville equation in terms of the classical force.

As $V(\mathbf{r})$ enters the Wigner kernel merely through the potential difference between the points $\mathbf{r}-\mathbf{x}/2$ and $\mathbf{r}+\mathbf{x}/2$, we express the latter as a line integral of the force along a path Γ from $\mathbf{r}-\mathbf{x}/2$ to $\mathbf{r}+\mathbf{x}/2$,

$$V\left(\mathbf{r}+\frac{\mathbf{x}}{2}\right) - V\left(\mathbf{r}-\frac{\mathbf{x}}{2}\right) = -\int_{\Gamma} \mathrm{d}\mathbf{s}\cdot\mathbf{F}(\mathbf{s})\,. \tag{3}$$

Note that, because $\mathbf{F}(\mathbf{s})$ is a conservative field, Γ can be any continuous curve connecting $\mathbf{r}-\mathbf{x}/2$ to $\mathbf{r}+\mathbf{x}/2$.

Next, we accommodate for the wave-like nature of quantum mechanics by decomposing the force in its plane wave components using the Fourier transform,

$$\mathbf{F}(\mathbf{r}) = \int \mathrm{d}^3k\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\tilde{\mathbf{F}}(\mathbf{k})\,. \tag{4}$$

Combining (3) and (4), we obtain a line integral over plane waves,