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A discontinuous Galerkin method for the Wigner-Fokker-Planck equation with a non-polynomial approximation space

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A discontinuous Galerkin approach to the Wigner-Fokker-Planck equation, a model for quantum devices including environmental effects, is proposed. Evaluation of a pseudo-differential term is the main challenge. The approach can be applied to a variety of potential functions and uses general approximation spaces. Simulations using the method are in agreement with established analytic results and produce reasonable solutions for several potentials.

1 Introduction

We report the implementation of a discontinuous Galerkin (DG) method for the Wigner-Fokker-Planck (WFP) equation,

$$w_t + k \cdot \nabla_x w - q\Theta[V](w) = Q_{FP}(w), \quad w(x,k,0) = w_0(x,k) \text{ s.t. } w_0, \mu^{-1} \in L^2\left(\mathbb{R}^2\right), \tag{1}$$

where μ is the stationary state when V is a harmonic potential [1, 2]. The equation describes the time evolution of the quasi-probability Wigner function $w(x,k,t)$ in the framework of open quantum systems, which accounts for interactions between the system and its environment [3, 4, 5]. The effects of a general potential V are embodied in the pseudo-differential operator,

$$\Theta[V](w(x,k,t)) = \frac{i}{\hbar\,(2\pi)^n} \int_{\mathbb{R}^{2n}} \left[V\left(x + \frac{\hbar}{m}\frac{\eta}{2}\right) - V\left(x - \frac{\hbar}{m}\frac{\eta}{2}\right)\right] w(x,p,t) \exp\left[i\eta \cdot (k-p)\right] d\eta dp,$$

where $\hbar$ is the scaled Planck constant. Environmental interactions are included in a Fokker-Planck diffusion type collision operator, $Q_{FP} = \Delta_k w + 2\mathrm{div}_k\left(kw\right) + \Delta_x w$.

The existence of smooth solutions to Equation 1 was proved in [6], including the case where V is determined by Poisson's equation. Recently, attention has turned to the existence and uniqueness of a nontrivial steady-state for potentials that are smooth perturbations of the harmonic potential, $V = \frac{1}{2}|x|^2 + V_0(x)$. In this case it is thought that any solution of the transient problem converges exponentially fast in time to the steady-state solution [2].

Previous numerical approaches to the problem include splitting methods [7, 8], finite differences [9], and recently the use of continued-fractions by Garcia-Palacios and Zueco [10, 11]. The potential strength of a DG implementation lies in its general applicability to a wide range of potentials and its accuracy, efficiency, and adaptability. Due to the highly oscillatory behavior of the solutions to the WFP equation, we used of non-polynomial approximation spaces, as proposed in [12]. This approach allows one to increase the resolution of the solution within each cell by tailoring the basis set to the particular problem. The method provides a setting in which the approximation space may be optimized to suit the specific features of the solution. Highly oscillatory solutions, which may arise near sharp changes in the potential, can be treated by adding oscillatory functions to the basis rather than refining the mesh. This method is also easily adapted to cases in which particularly good approximation spaces are known, such as the use of Hermite functions in cases related to the harmonic oscillator.

2 Notation and Implementation

The Wigner function is projected into a space spanned by the set $\left\{\phi_{(j,m)}(x,k) = \mathcal{X}_{(j,m)}(x)\mathcal{K}_{(j,m)}(k)\right\}_{j=0}^{N}$, where each basis function is supported in a single cell. The primitive basis functions, $\mathcal{X}_j(x)$ and $\mathcal{K}_j(k)$ can vary from polynomials to trigonometric or Hermite functions. Computational complexity is reduced if the primitive basis functions are orthogonal, and, if the orthogonality is not natural the Gram-Schmidt procedure is applied to the basis.

A standard third-order total variation diminishing Runge-Kutta method is used for time integration [13]. The transport term is discretized following the same procedure as found in [14]. The elliptic part of the collision operator is approximated using a non-symmetric interior penalty method (the so called NIPG method) as in [15]. The main contribution of this work is the method for numerical evaluation of the pseudo-differential operator Θ. The operator contains an infinite oscillatory integral over η, which can be difficult to evaluate for unbounded $V(x)$. However, the pseudo-differential operator has an especially convenient expression in the case of a harmonic potential,

$$\Theta[V_0|x-a|^2](w) \quad = \quad -2\frac{V_0}{m}(x-a)\cdot\nabla_k w. \tag{2}$$

A series representation of the pseudo-differential operator is available that only contains the products $\nabla_x^b V(x) \cdot \nabla_k^b w(x,k,t)$ of odd order b. The series is ideal for the harmonic term in the potential, however, it is difficult to treat higher order derivatives in the DG framework. We take advantage of the linearity of the operator and treat the harmonic part of the potential with equation 2 and the bounded part with the integral representation. When the test function is replaced with a basis function, the basic integrals (summation and scaling factors are suppressed) in the weak form of the pseudo-differential operator,

$$\left(\Theta[V](w), \phi_{(l.m)}\right) = i \int \int_{\Omega_l} \int_{\partial\Omega_l^x} \int_{\mathbb{R}} DV\,(x,\eta)\,\phi_{(l,n)}(x,p)\phi_{(l,m)}(x,k)\exp\left[i\eta(k-p)\right] d\eta dp dx dk.$$

where $DV(x,\eta) = V\left(x + \frac{\hbar\eta}{2m}\right) - V\left(x - \frac{\hbar\eta}{2m}\right)$, contain two Fourier transforms of the basis functions. These transforms are calculated analytically to reduce computational cost. We remark that the restriction to cell Ω_j ruins periodicity, but that the transform is still simple. The use of Hermite functions is more technically complicated, but possible. A purely numerical approach, while more computationally intensive, is available in case that the potential contains higher order unbounded terms. The integral representation of the operator can be used in these cases, but the integral over η, while finite, can be highly oscillatory and extremely slow to converge. Oscillatory methods are required in these situations. A test case, in which the integral representation of the operator was evaluated for a harmonic potential and trigonometric basis functions, was solved by taking a multiscale approach. A simple but effective method was constructed in the framework of the Heterogeneous Multiscale Methods [16] in which the value of the integral over the real line was extrapolated from the evaluation of the integral over a widely dispersed set of short intervals.

The method has been implemented and tested by selecting several sub-problems contained in equation 1. The tests verify that the method correctly solves the transport and heat equations as well as sustaining the steady state Gaussian solution of the harmonic oscillator (i.e. the zeroth order Hermite function). A test to verify the full WFP equation using the harmonic potential confirms the results of Sparber et al. [1] in that the solution shows exponential decay in the L^2 norm to a steady state (while preserving mass) as shown in Figure 1.

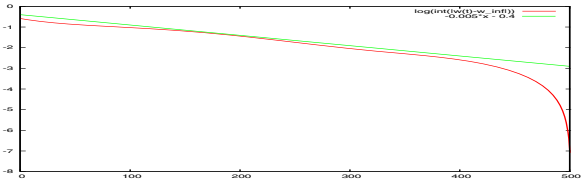

Fig. 1 Exponential decay to steady state (approximated by $w(x,k,t)$). The graph shows the difference $|w(x,k,t) - w(x,k,T)|_2^2$ as a function of t on a log scale alongside a reference line with slope -0.005.

The program has also been used with non-harmonic potentials to test the integral representation of the pseudo-differential equation. Step potentials and smooth box potentials (a pair of steep adjacent Gaussian potentials) have shown correct qualitative behavior. The expected exponential decay to a steady state for perturbations of the harmonic potential is also observed [2].

Currently, the code is being used to aid the analysis of a modification of the WFP problem.

The non-polynomial DG method provides a setting to optimize the approximation space to suit the specifics of the problem. Highly oscillatory solutions may arise near a sharp change in the potential, at which point oscillatory functions could be added adaptively to achieve subgrid resolution. In cases where good approximation spaces are available, such as the use of Hermite functions in cases related to the harmonic oscillator, the non-polynomial approach is easily adapted.

Future work will include this optimization as well as extension of the code to general meshes in higher dimensions.

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