USING THE NAG TOOLBOX TO SOLVE NUMERICALLY A NONLINEAR FOURTH-ORDER QUANTUM DIFFUSION EQUATION

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The ongoing trend of increasing miniaturization in nanotechnology has now reached the borders where classical models can be applied for device simulations and is entering the nanoscale domain (cca. 10 nm) where quantum effects can no longer be neglected. Novel models are therefore required which incorporate these quantum effects. Starting from basic quantum principles, a whole hierarchy of quantum fluid-type models has been derived.

One of the simplest quantum models is the quantum drift-diffusion (density gradient) model, in which certain quantum effects are modelled by the fourth-order nonlinear parabolic (quantum diffusion) equation

$$\partial_t n = -\operatorname{div}\left(n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\right), \tag{1}$$

where n denotes the particle density (e.g. electrons in semiconductors). Equation (1) admits particular variational structure. Namely, the variational derivative of the Fisher information functional $F[n] = \int |\nabla\sqrt{n}|^2 \mathrm{d}x$ equals $\delta F[n]/\delta n = -\Delta\sqrt{n}/\sqrt{n}$ and, imposing appropriate boundary conditions, dissipation of the Fisher information along each trajectory solution of (1) follows immediately:

$$\frac{\mathrm{d}}{\mathrm{d}t}F[n(t)] = -\int n\left|\nabla\frac{\delta F[n]}{\delta n}\right|^2 \mathrm{d}x \le 0.$$

From a numerical and applicational point of view, it is a desirable and challenging task to construct reliable numerical schemes which preserve the variational structure, the dissipation property and other structural properties of the equation on a discrete level.

The key idea of the discrete variational derivative method (DVDM) is to define a discrete analogue (approximation) F_d of the Fisher information and to perform a discrete variation procedure in order to obtain the discrete variational derivative $\delta F_{\mathrm{d}}/\delta(U^{k+1},U^k)$, the discrete analogue of $\delta F[n]/\delta n$. The method is then given by the nonlinear system

$$\frac{1}{\tau}(U^{k+1}-U^k) = \delta^{\langle 1\rangle}_{\mathrm{div}}\Big(U^{k+1}\delta^{\langle 1\rangle}_{\mathrm{grad}}\Big(\frac{\delta F_{\mathrm{d}}}{\delta(U^{k+1},U^k)}\Big)\Big)\,, \quad k \geq 0\,, \tag{2}$$

where the real vector of unknowns U^k approximates the exact solution n on the time-level t_k and a given spatial grid. Discrete differential operators $\delta^{\langle 1\rangle}_{\mathrm{div}}$ and $\delta^{\langle 1\rangle}_{\mathrm{grad}}$ are defined so that (2) is consistent with (1). Method (2) is a discrete analogue of (1) which, by construction, preserves the variational structure and, imposing corresponding discrete boundary conditions, it also preserves mass and the dissipation property of the Fisher information, i.e. $F_{\mathrm{d}}[U^{k+1}] \leq F_{\mathrm{d}}[U^k]$ for all $k \geq 0$.

In order to solve the nonlinear system (2) numerically, the NAG toolbox routine `c05nb`, based on a modification of the Powell hybrid method for nonlinear systems, has been employed. This routine proved to be approximately three times faster than the standard MATLAB routine `fsolve` and because of that it was extremely useful for executing all required numerical tests and experiments in reasonable time.

The above roughly presented discrete variational derivative method and related numerical results are part of the author's PhD thesis "Entropy analysis for nonlinear higher-order quantum diffusion equations", which has been done at the Vienna University of Technology under supervision of Prof. Ansgar Jüngel.

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