Karlsruher Institut für Technologie

Scientific Computing Center

Neural Operators for Quantum Transport:
Learning Wigner Dynamics Across the Semiclassical Regime

Target group

M.Sc. Mathematics / Computational and Data Science

Description of the topic

Context. Quantum transport is important in semiconductor physics, nanoelectronics, and microscopic particle systems. The Wigner equation describes collisionless quantum dynamics in phase space. In one spatial dimension, using nondimensional variables and unit mass, it reads

$$\partial_t W^\varepsilon + p\,\partial_x W^\varepsilon = \Theta_\varepsilon[V]W^\varepsilon, \qquad W^\varepsilon(0,x,p) = W_0^\varepsilon(x,p).$$

Here x is position, p momentum, $\varepsilon > 0$ the semiclassical parameter, and $\Theta_\varepsilon[V]$ the nonlocal quantum potential operator for a potential $V(x)$. Wigner functions can take negative values and exhibit interference; the dynamics can be strongly oscillatory.

Neural operator learning. Neural operators, such as Deep Operator Networks (DeepONets), learn mappings between functions. They can approximate solution operators for families of potentials and wave-packet initial states. Their effectiveness for oscillatory quantum transport is an open computational question.

Classical limit and hybrid approximation. For smooth potentials and fixed, sufficiently regular test functions f, the formal leading term of $\Theta_\varepsilon[V]f$ as $\varepsilon \to 0$ is $V'(x)\partial_p f$. This motivates a Liouville baseline:

$$\partial_t W_{\mathrm{cl}}^\varepsilon + p\,\partial_x W_{\mathrm{cl}}^\varepsilon - V'(x)\,\partial_p W_{\mathrm{cl}}^\varepsilon = 0, \qquad W_{\mathrm{cl}}^\varepsilon(0) = W_0^\varepsilon.$$

It transports the same, possibly signed initial Wigner data. We propose the hybrid approximation

$$\widehat{W}_\theta^\varepsilon(t,x,p) = W_{\mathrm{cl}}^\varepsilon(t,x,p) + \mathcal{N}_\theta[W_0^\varepsilon, V, \varepsilon](t,x,p),$$

where a neural operator $\mathcal{N}_\theta$ approximates the quantum correction and is constrained to vanish at $t = 0$. In computations, the Liouville baseline is approximated numerically; residual learning may also absorb its discretization error. The formal limit does not guarantee a uniformly small correction for oscillatory, ε-dependent data. Capturing interference and tunneling accurately across semiclassical regimes is a central research question.

The project combines mathematical analysis, operator learning, and numerical simulation of quantum transport, with initial experiments possible in one spatial dimension.

Helpful prerequisites

- Numerical analysis of differential equations
- Linear algebra and functional analysis
- Interest in quantum mechanics or kinetic theory
- Machine learning experience

Exemplary research questions

- Can a neural operator approximate Wigner dynamics for families of potentials and initial conditions?
- Can the classical limit be exploited to improve approximation accuracy and generalization?
- How does accuracy depend on the semiclassical parameter and potential complexity?
- Can a hybrid neural-classical method reproduce tunneling and interference more reliably than an unconstrained neural operator?
- How do accuracy, stability, training cost, and prediction cost compare with spectral solvers?

Scope. The initial goal is to simulate wave packets interacting with smooth potential barriers and develop and evaluate the hybrid method. Error estimates or uniform approximation across semiclassical regimes are possible extensions, depending on the student's background.

Contact

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