Gaussian-process-regression-based method for the localization of exceptional points in complex resonance spectra

P. Egenlauf¹, P. Rommel^{1,*}, J. Main¹

¹Institute for Theoretical Physics I, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany. *patric.rommel@itp1.uni-stuttgart.de

Resonances in open quantum systems depending on at least two controllable parameters can show the phenomenon of exceptional points (EPs), where not only the eigenvalues but also the eigenvectors of two or more resonances coincide. Their exact localization in the parameter space is challenging, in particular in systems, where the computation of the quantum spectra and resonances is numerically very expensive. We introduce an efficient machine learning algorithm to find EPs based on Gaussian process regression (GPR) [1]. The GPR-model is trained with an initial set of numerically determined eigenvalue pairs belonging to an EP and used for a first estimation of the EP position via a numerically cheap root search over the model output. The estimate is then improved iteratively by adding selected exact eigenvalue pairs, typically calculated at the currently estimated EP position, as training points to the GPR-model. The GPRbased method is developed and tested on a simple low-dimensional matrix model and then applied to a challenging real physical system, viz., the localization of EPs in the resonance spectra of excitons in cuprous oxide in external electric and magnetic fields. The precise computation of EPs, by taking into account the complete valence band structure and central-cell corrections of the crystal, can be the first step towards an experimental realization of EPs in this system.



Fig. 1. When an exceptional point is circled in the space of the complex parameter κ , the corresponding eigenvalues exchange their positions in the complex λ plane.

References

[1] P. Egenlauf, P. Rommel, J. Main, Machine Learning: Science and Technology 5, 015045, (2024).

Acknowledgements

This work was supported by Deutsche Forschungsgemeinschaft (DFG) through Grant No. MA 1639/16-1.