Application of machine learning methods in the targeted energy transfer nonlinear model

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The Targeted Energy Transfer (TET) mechanism involves resonant transfer of energy in a non-resonant but nonlinear system [1]. The original idea was motivated by ultrafast electron transfer in chlorophyl molecules and was formulated in the context of the Discrete Nonlinear Schroedinger (DNLS) equation. The transfer is perfect when a specific constrain is fulfilled that connects nonlinearity with energy disparity in the context of a two state model. While it applies to classical models it can be readily extended to quantum systems as well [2]. In both classical and quantum cases it is very important to find the constrain that enables efficient transfer. While this is possible in simple dimer units it becomes a very challenging task in more extended systems. In order to bypass this difficulty we may apply techniques from Machine Learning (ML). Specifically, by selecting appropriate loss function and minimising it in the system parameter space one may obtain a direct formulation of the appropriate constrain that leads to resonant transfer. In the classical oscillator case we can find easily the TET transfer condition by employing this method in the dimer case that is known analytically [3]. Furthermore, we can use the method in more complex geometries such as the a trimer that involves a nonlinear dimer unit that is separated by a linear state. While this trimer model is not analytically tractable the application of the ML approach gives readily the resonant transfer parameter landscape. Similar approach can be applied to the quantised version of the DNLS model [4]. Extension of the classical loss function to the quantum case and subsequent minimisation through learning and back-propagation results in the precise analytical TET result for the quantum system. The method is then applied to the fully quantum trimer case where the intermediate stat is in general nonlinear. Assuming that two of the oscillators fulfil the quantum TET condition leads to optimisation of transfer through the third state. This transfer enables movement of arbitrary number of bosons in unison from the donor to the acceptor state. The successful application of ML techniques in this model is now being extended to the cases where in addition to the electronic degrees of freedom we also have vibrational degrees as well [5]. We show analytically and numerically that TET works quite efficiently also in this more complex case. We focus on the temperature dependence of the phenomenon and apply our ML technique in order to find parameter regimes for optimal transfer. In conclusion the TET model is quite general and through the application of ML methods one may uncover its full applicability.

References

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