Variational error in molecular quantum dynamics — a dialog between maths and chemistry

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In this talk we shall discuss how to handle estimates of the variational error inherent to simulations in molecular quantum dynamics from the joint perspective of mathematical physics and physical chemistry. In this context, scale identification is common practice, especially within the context of the electronic-nuclear Born-Oppenheimer approximation, but also for uncorrelated approximations relying on a vibrational system-bath type partitioning. This will be illustrated on the prototypical case of a two-mode system experiencing tunnelling along a reaction coordinate and a cubic coupling with a harmonic bath [1,2].

[1] I. Burghardt, R. Carles, C. Fermanian Kammerer, BL, and C. Lasser, J. Phys. A 54 (2021) 414002
[2] I. Burghardt, R. Carles, C. Fermanian Kammerer, BL, and C. Lasser, J. Phys. A 55 (2022) 224010.