

# Hagedorn Wave packets and Time-Dependent Schrödinger Equation on non-adiabatic molecular dynamic: ground and excited states.

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## ABSTRACT

The simulation of molecular quantum dynamics is done by numerically solving the time-dependent Schrödinger equation (ES). There are several ways to represent the mathematical solution of ES. The traditional way of representing this solution is to project it on a time-independent basis. Another way is to represent it on a time-dependent basis. In this last category, there are several simulation techniques such as MCTDH [3], HELLER [2], vMCG[4], HAGEDORN [1] etc... For the Hagedorn technique, like the rest of the techniques in this category, the basis moves over time following the evolution of the wave packets. This way of carrying out propagation makes it possible to optimally reduce the number of primitive basis functions. Subsequently, this way of doing things also makes it possible to delay exponential growth. We also save time and IT resources

## References

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