

A Time-Dependent Born-Oppenheimer Approximation with Exponentially Small Error Estimates

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We present joint work with Alain Joye on the construction of an exponentially accurate time-dependent Born–Oppenheimer approximation for molecular quantum mechanics.

We study molecular systems whose electron masses are held fixed and whose nuclear masses are proportional to ϵ^{-4} , where ϵ is a small expansion parameter. By optimal truncation of an asymptotic expansion, we construct approximate solutions to the time-dependent Schrödinger equation that agree with exact normalized solutions up to errors whose norms are bounded by $C \exp(-\gamma/\epsilon^2)$, for some C and $\gamma > 0$.