Mathematical Physics

On the divergence of time-dependent perturbation theory applied to laser-induced molecular transitions: Analytical calculations for the simple algorithm

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Shaped laser pulses are a powerful tool to induce population transfer between electronic molecular states, and time-dependent perturbation theory is suitable for a description of such a transfer in weak external fields. The application of perturbation theory in numerical simulations of field matter interactions can lead to divergences. In a recent paper [K. Renziehausen et. al., J. Phys. B: At. Mol. Opt. Phys., 42:195402, 2009] we explained that the arising error in the norm of the wave function can be split into two parts. The first part is related to numerical errors caused by the discretisation of time that is required in the simulation and can be suppressed for a sufficiently small time step or abolished for an adequate numerical implementation of perturbation theory. The second part may cause divergences and is associated with the perturbative expansion order. We presented numerical evidence without any analytical proof. Here we are focussing on the derivation of analytical expressions to interpret the behavior of what we have called in the above mentioned paper 'simple algorithm'. The derivation of analytical expressions for the interpretation of what we have called in the above mentioned paper 'improved algorithm' are given in another paper [K. Renziehausen. arXiv, in preparation, 2012]. Moreover, we introduce here a gedankenexperiment to illustrate the influence of the different orders on the field-molecule interaction.

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