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# Adiabatic perturbation theory for atoms and molecules in the low frequency regime


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Abstract

The possibility to create extremely short pulses, using high-order harmonics created by a low-frequency driving field, has stimulated studies of photo induced dynamics in the low-frequency regime. Using low-frequency driver lasers for high-order harmonic generation (HHG) is attractive because the cut-off limit scales as one over the laser frequency squared. However, the low frequency raised challenges in dynamics calculation in this regime.The multiphoton absorptions by molecules in strong laser fields depend on the polarization of the laser and on the molecular structure.

We represent a perturbational approach for the calculations of the quasi-energy spectrum in the low frequency regime, that avoids the construction of the Floquet operator with extremely large number of Floquet channels. The zero-order Hamiltonian in our perturbational approach is the adiabatic Hamiltonian where the atoms/molecules are exposed to a dc electric field rather than to ac-field. The second order perturbation correction terms are obtained when $-i\hbar\omega\frac{\partial}{\partial\tau}$ serves as a perturbation and $\tau$ is a dimensionless variable.

The second order adiabatic perturbation scheme is found to be an excellent approach for calculating the ac-field Floquet solutions in our test case studies of a simple one-dimensional time-periodic model Hamiltonian. It is straightforward to implement the perturbation approach presented here for calculating atomic and molecular energy shifts (positions) due to the interaction with low frequency ac-fields using high-level electronic structure methods. This is enabled since standard quantum chemistry packages allow the calculations of atomic and molecular energy shifts due to the interaction with dc-fields. In addition to the shift of the energy positions the energy widths (inverse lifetimes) can be obtained at the same level of theory.


**ההרצאה תתקיים ביום רביעי, ה-6.6.18 בשעה 12:30**
**באודיטוריום המכון למצב מוצק, קומת כניסה**
**The lecture will take place on Wednesday, 6.6.18 at 12:30**
**at the Solid State Institute auditorium, entrance floor**

Ph.D. Student of Professor Nimrod Moiseyev