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Non-linear Stark Effect and Molecular Localization

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Abstract. We consider a non-linear Stark effect as a model for localization and symmetry breaking of a molecule in a gas. By a comparison method with respect to the linear Stark effect, we prove the existence of level bifurcation and symmetry breaking at a critical value of the gas pressure exponentially small for large nuclear masses. Extending the Davies results, we confirm the predictions of Claverie-Jona Lasinio for pyramidal molecules as the ammonia one.

0 Introduction

The empirical chemical models for molecules imply certain asymmetries and structures in apparent contradiction with quantum mechanical principles. Even the accepted features of the water molecule [Pr] are not proved to be in agreement with straightforward application of quantum mechanics. One possible explanation of this phenomenon lies on the existence of non-stationary states that are more stable than the stationary ones to the environment interactions.

As a particularly interesting example of molecule with structure we have the ammonia one NH_3 (or AsH_3, PH_3). To be more clear, following Wightman [Wi], it is better to consider the similar molecule NHDT (or AsHDT, PHDT) in which the three hydrogen nuclei are distinguished by isotopes. Such molecules have a pyramidal structure with the HDT in a triangular basis and the N in the vertex. Actually there are two kinds of such pyramides with different chirality. Chiral molecules can be discovered by the "optical activity": they are able to rotate the polarization plane of light. Quantum mechanics predicts symmetrical molecules with the N nucleus delocalized in both possible vertices. In the Born-Oppenheimer approximation the N nucleus feels a double well potential as it is clear since 1927 [Ha]. Quantum levels are split in two because of the two possible even/odd inversion states. States initially localized in one well (chiral states) oscillate (beating effect) from one well to the other. Physically we always observe stable (without oscillations) chiral molecules in a gas at a pressure large enough (at fixed temperature). All the models used for