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The Role of Size and Shape in the Stability of the Quantum Brownian Rotator

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Shape and size are the basic characteristics of macroscopic, classical systems, and as such represent a special challenge within the fundamental problem of "transition from quantum to classical", but also the problem of quantum measurement. Propeller-shaped molecules are excellent candidates for analyzing the effects of size and shape because of the linear dependence of both the moment of inertia and the damping factor on the number of propeller blades. Also, such research can be useful for their practical application within molecular machines technology [1,2].

The propeller-shaped large-molecules rotators can be modeled by a single (rotational) degree of freedom as a rigid system that is open to the environmental influence using the so-called Caldeira-Leggett master equation [3]. The use of this equation is motivated by both, the well-defined classical limit as well as by the explicit quantummechanical corrections in the weak-coupling limit, although it was used phenomenologically. Two methods for investigating stability are used, a quantum-mechanical counterpart of the so-called "first passage time"method, and investigation of time dependence of the standard deviation of the rotator for both the angle and angular momentum quantum observables. The analysis was performed for three different cases of external potential, the free, harmonic and weakly nonharmonic rotator [4,5].

The analysis of the dynamics of molecular propellers showed the presence of quantum corrections that are not negligible, especially in short initial time intervals. It was concluded that in the transition from quantum to classical dynamics in the case of molecular propellers, contrary to expectations, quantum decoherence is not the dominant process [4,5].

A number of interesting theoretical predictions regarding stability of rotation are obtained: for certain parameter regimes the time decrease of the standard deviations and also nonmonotonic dependence on the rotator size are observed for the standard deviations and for the damping of the oscillation amplitude, which is contrary to the classical expectation that the size of the rotator can be reduced to the inertia of the rotator [4,5].

The sensitivity of rotation to details of the model and the parameter regimes emphasizes that utilizing the propeller rotations stability is an optimization problem that requires a separate careful analysis.

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