Tunneling Quantum Dynamics in Ammonia

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Ammonia is a well-known example of a two-state system and must be described in quantum-mechanical terms. In this article, we will explain the tunneling phenomenon that occurs in ammonia molecules from the perspective of trajectory-based quantum dynamics, rather than the usual quantum probability perspective.

Keywords: ammonia ; quantum molecular dynamics ; quantum Hamilton mechanics ; tunneling dynamics ; quantum trajectory

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1. Introduction

Tunneling, one of the most fascinating and mysterious phenomenon in the microscopic world, has benefitted our daily life for decades. Even though quantum mechanics has provided some useful information about tunneling, we still barely know how it works. As new technology equips quantum devices with more potential advanced usages and applications [1][2][3][4], the current knowledge has reached its limitation. More studies have begun to extend this limitation to the edge of the microscopic world [5][6][7][8]. To seek the underlying physics and mechanism of tunneling, various approaches have been studied [9][10][11][12][13][14][15][16][17][18][19][20]. One of these approaches is the trajectory interpretation of quantum mechanics, which regards the wave function as an ensemble of trajectories [21][22][23][24][25][26][27][28].

The trajectory interpretation of quantum mechanics provides an ontological perspective to view the microscopic world. By means of an ensemble of trajectories, particle properties and wave properties in quantum theory can be connected [29][30]. In recent years, the discussion of the quantum trajectory has been extended to the complex space [31][32][33][34][35][36]. Higher dimensions provide leverage in tackling unsolved quantum issues and explaining more quantum phenomena [37][38][39][40][41][42][43][44][45][46]. Underlying the framework of complex trajectory interpretation, tunneling dynamics have been provided and studied. Levkov [47] closely inspected tunneling trajectory in a chaotic model in the complex domain. Yang [48] presented tunneling dynamics in the complex space, revealing a smooth trajectory which continuously connects the classical trajectory and tunneling trajectory. John [49] evaluated the reflection probability in terms of the reflected and incident complex trajectories.

A series of experiments verify the reality of quantum trajectories, and some even show the importance and necessity of the consideration of the complex domain in the quantum system [50][51][52][53][54][55][56]. Following the proposal of a weak value [57], the measurement and observation of the quantum system can be carried out to reveal the reality of the quantum realm. Under the minimum degree of interference in the quantum system, this weak measurement endows the complex eigenvalues with the physical meanings. Various researches have extensively studied the fundamental mechanisms of the weak value, pointing out that the imaginary part of the weak value is significantly important to quantum observations [58][59][60][61][62]. In the latest research, this complex number is reported as an essential element in inspecting quantum systems [63][64]. With support from both theoretical and experimental evidences, the complex trajectory interpretation is gradually becoming one of the most conceivable interpretations of quantum mechanics. In the present research, we will apply the complex trajectory interpretation to a practical quantum system involving ammonia and its inversion state in order to analyze the tunneling dynamics between them.

Ammonia is formed in the shape of a pyramid, with three hydrogen atoms situated on an equilateral triangle plane with the nitrogen atom on the apex. The pyramid inverts as the nitrogen atom changes position from one equilibrium point to another via the tunneling effect. This inversion flip-flops repeatedly with the tunneling rate

Hz, which is calculated by solving the Schrödinger equation in the double-well potential with the WKB method [65], having an experimental value of 2.3786 * 10 ^10 Hz.

From the viewpoint of quantum mechanics, it is probably that at a given time the nitrogen atom is situated on either side of the equilateral triangle plane formed by the three hydrogen atoms. In other words, it is partly on both sides at the same time in a quantum mechanical sense. However, the frequency of the nitrogen atom flips back and forth has been experimentally observed [66]. Does this imply that the nitrogen atom is wholly on one side or on the other at any given instant? In this paper, we will analyze the tunneling dynamics in ammonia by means of the complex trajectory interpretation of quantum mechanics. It seems that the tunneling trajectory might provide some convincing answers to the above question.

2. Tunneling Quantum Dynamics in Ammonia

Quantum Hamilton mechanics provides a remarkable deterministic way to explore tunneling dynamics in ammonia. The magic phenomenon that a nitrogen atom with insufficient kinetic energy can pass through the potential barrier in ammonia now becomes understandable by tracing the trajectory of the nitrogen atom. We found that the quantum potential plays the most important role in tunneling dynamics by creating a tunneling channel in the complex plane for the nitrogen atom to pass through. The tunneling phenomenon as traditionally described in the language of probability can now be described in more detail through the motion of the nitrogen atom in a complex plane.

Complex tunneling trajectories in both the stationary states and the two-level transition state in the double-well potential have been studied here. Tunneling dynamics in stationary states have an analytical expression and help us to describe the tunneling phenomenon concisely. However, the computed tunneling frequency and tunneling range in the stationary states have a significant deviation from the experimental data. Compared to the stationary states, the two-level transition state provides a more accurate description of the tunneling process, if the double-well potential is used. In the two-level state, we find that a tunneling channel that moves with time in the complex plane appears in the total potential. It is through this moving channel that the nitrogen atom travels back and forth between the ammonia state and the ammonia inversion state. The tunneling frequency, 24.35 GHz, computed from the complex trajectory of the nitrogen atom, is close to the measured frequency of 23.8 GHz. As to the tunneling range, the measured value is 0.38A, however our analysis shows that the tunneling ranges on the two states should be different. The reason is that the potential barrier in the ammonia inversion state is slightly higher than that in the ammonia state and thus it is harder for the nitrogen atom to penetrate. Accordingly, the tunneling range in the ammonia inversion state is found to be 0.294A, which is slightly shorter than that in the ammonia state, which is found to be 0.30175A. This asymmetric apex arises from the experimental observed energy split of the ammonia state and its inversion state. In this study, we analyze the transition between the two states in detail and propose a theoretical result of the different tunneling ranges in the two states. Hopefully, this study can provide some useful information for related experiments.

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