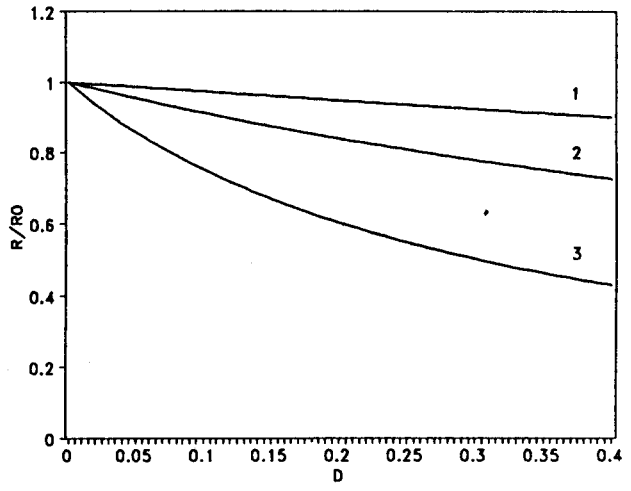

Figure 4. The ratio of R/R_0 for the bistable system with $\nu=0.2$. The curves 1, 2, and 3 correspond to $\mu=0.5$, $\mu=1$, and $\mu=2$, respectively.

and $\nu=0.9$, respectively. In Figure 4 we have taken μ to be 0.5, 1, and 2, respectively, when $\nu=0.2$. As D increases the ratio in large μ value decreases faster than the ratio in small μ does. As shown in Figure 3, it is obvious that in the region $\nu<1$ the transition rates decrease with increasing D. As the exponent ν increases, the transition rates decrease and relaxation times increase. In the limit $\nu\rightarrow1$, the transition rate approaches zero.

In the result, in the region for which $\nu<1$ the transition rates decrease as ν increases and ν decreases shown in Figure 3 and 4. However, in the case that $\nu>1$, it is obvious that in Eq. (17) never probability can be reach $y\rightarrow\infty$ in any finite time. It means that the system cannot be reach the unstable state since the concentration $x\rightarrow0$ (unstable point) corresponds to $y\rightarrow\infty$. When $\nu>1$ the random force is so weak that the system is entirely controlled by the deterministic term in the vicinity of the unstable state. The transition between the two deterministic stable states cannot occur and the initial distribution is continuously retained.

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Orbital Interactions in BeC_2H_2 and LiC_2H_2 Complexes

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Ab initio calculations are carried out at the 6-311G** level for the C_{2v} interactions of Be and Li atoms with acetylene molecule. The main contribution to the deep minima on the $^3B_2$ BeC_2H_2 and $^2B_2$ LiC_2H_2 potential energy curves is the b_2 ($2p(3b_2)-|\pi_g^*(4b_2)$) interaction, the a_1 ($2s(6a_1)-|\pi_u(5a_1)$) interaction playing a relatively minor role. The exo deflection of the C-H bonds is basically favored, as in the b_2 interaction, due to steric crowding between the metal and H atoms, but the strong in-phase orbital interaction, or mixing, of the a_1 symmetry hydrogen orbital with the $5a'_1$, $6a'_1$ and $7a'_1$ orbitals can cause a small endo deflection in the repulsive complexes. The Be complex is more stable than the Li complex due to the double occupancy of the $2s$ orbital in Be. The stability and structure of the MC_2H_2 complexes are in general determined by the occupancy of the singly occupied frontier orbitals.

Introduction

The interactions of metal atoms with molecules have been the subject of many experimental and theoretical studies.[1] The main purpose of the research in this field is a fundamental understanding of catalysis. It has been suggested that