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Diffusion of a particle on a static rugged energy landscape with spatial correlations BIMAN BAGCHI, SAIKAT BANERJEE, Indian Institute of Science — Despite the broad applicability of the problem, we have limited knowledge about the effect of ruggedness on diffusion at a quantitative level. Every study seems to use the expression of Zwanzig [Proc. Natl. Acad. U.S.A, 85, 2029 (1988)] who derived the effective diffusion coefficient, $D_{eff} = D_0 \exp\left(-\beta^2\varepsilon^2\right)$. We introduce and study two models of Gaussian random energy surface; a discrete lattice and a continuous field. Our simulations show that Zwanzig's expression overestimates diffusion in the uncorrelated Gaussian random lattice. The disparity originates from the presence of "three-site traps" (TST) on the energy landscape – which are formed by the presence of deep minima flanked by high barriers on either side. Using mean first passage time (MFPT) formalism, we derive a general expression for the effective diffusion coefficient, $D_{eff} = D_0 \exp\left(-\beta^2\varepsilon^2\right)\left[1 + \mathrm{erf}\left(\beta\varepsilon/2\right)\right]^{-1}$ in the presence of TST. In presence of spatial correlation we derive a more general form of the expression, which reduces to Zwanzig's form in certain limits. We characterize the same using non-Gaussian order parameter, and show that this "breakdown" scales with ruggedness following an asymptotic power law. The breakdown of Zwanzig's elegant expression was perhaps anticipated but was not clearly demonstrated earlier.

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