

Vineyard Prefactor

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The dynamical matrix at the initial point is H° , and the dynamical matrix at the saddle is H^\dagger . Let $S(A)$ be the sequence of eigenvalues of A , and let $\tilde{S}(A) = \{\lambda : \lambda \in S(A) \text{ and } \lambda > 0\}$. Then, the Vineyard prefactor is:

$$\nu = \frac{\prod_{\lambda \in S(H^\circ)} \sqrt{\lambda}}{\prod_{\lambda \in \tilde{S}(H^\dagger)} \sqrt{\lambda}} \quad (1)$$

Or, equivalently:

$$\nu = \exp \left(\frac{1}{2} \left(\sum_{\lambda \in S(H^\circ)} \ln \lambda - \sum_{\lambda \in \tilde{S}(H^\dagger)} \ln \lambda \right) \right) \quad (2)$$

This definition avoids the overflow from multiplying many numbers together.

Note that here we define the dynamical matrix with elements with $1/\text{time}^2$ units.