

# rmgpy.kinetics.Wigner

`class rmgpy.kinetics.Wigner(frequency)`

A tunneling model based on the Wigner formula. The attributes are:

Attribute	Description
<i>frequency</i>	The imaginary frequency of the transition state

An early formulation for incorporating the effect of tunneling is that of Wigner [1932Wigner]:

$$\kappa(T) = 1 + \frac{1}{24} \left( \frac{h |\nu_{\text{TS}}|}{k_{\text{B}} T} \right)^2$$

where  $h$  is the Planck constant,  $\nu_{\text{TS}}$  is the negative frequency,  $k_{\text{B}}$  is the Boltzmann constant, and  $T$  is the absolute temperature.

The Wigner formula represents the first correction term in a perturbative expansion for a parabolic barrier [1959Bell], and is therefore only accurate in the limit of a small tunneling correction. There are many cases for which the tunneling correction is very large; for these cases the Wigner model is inappropriate.

**calculate\_tunneling\_factor(*self*, *double T*)** → *double* ¶

Calculate and return the value of the Wigner tunneling correction for the reaction at the temperature  $T$  in K.

**calculate\_tunneling\_function(*self*, *ndarray Elist*)** → *ndarray*

Raises `NotImplementedError`, as the Wigner tunneling model does not have a well-defined energy-dependent tunneling function.

**frequency**

The negative frequency along the reaction coordinate.

[1932Wigner] E.Wigner. *Phys. Rev.* **40**, p. 749-759 (1932). doi:10.1103/PhysRev.40.749

[1959Bell] R. P. Bell. *Trans. Faraday Soc.* **55**, p. 1-4 (1959). doi:10.1039/TF9595500001