8.2 Detailed balance condition and Metropolis algorithm

Thermodynamic equilibrium describes stationary macro-states, while the micro-states still change continuously. To allow for this macro-state-stationarity the changes between micro-states must obey the so called detail balance condition, i.e. the probability for the transition from micro-state l into micro-state m must be identical to the probability for the transition from micro-state m into micro-state l. We will discuss briefly the Metropolis algorithm; it fulfills the detailed balance condition, thus allowing to simulate thermodynamic equilibrium, and in addition it correctly simulates the "path" into thermodynamic equilibrium, i.e. many transport and scattering phenomena.
In each iteration step of the Metropolis algorithm the probability $p_{l\to m}$ is calculated for replacing the old parameter value v_l by the new parameter value v_m. For this the overall energies $E_l(v_l)$ and $E_m(v_m)$ are calculated. If $E_m < E_l$ the replacement will be accepted. Otherwise

$$p_{l\to m} = \exp\left(-\frac{E_m - E_l}{k\,T}\right) \tag{8.1}$$

is calculated, a random number $0 < x_{random} < 1$ is calculated, and the replacement will be accepted if $x_{random} < p_{l\to m}$. In principle $k\,T$ is an arbitrary positive number, but of course T has the physical meaning of a temperature, i.e. taking larger values of T replacements will be accepted more often even if the over all energy is increasing.