

统计力学及应用作业 3

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证明 Metropolis 方法产生的随机数列分布为 $\rho(x)$, 若 $\frac{A_{xx'}}{A_{x'x}} = \frac{\rho(x')}{\rho(x)}$.

讲过长时间的发展后, 处于某一状态 x 的概率都为常数. 考虑 x, x' 两点间转化的概率, 不妨设 $\rho(x) > \rho(x')$.

$$T(x \rightarrow x') = \omega_{xx'} A_{xx'} = \omega_{xx'} \frac{\rho(x')}{\rho(x)}, \quad (1.1)$$

$$T(x' \rightarrow x) = \omega_{x'x} A_{x'x} = \omega_{x'x}. \quad (1.2)$$

由于

$$T(x \rightarrow x')\rho(x) = \omega_{xx'} \frac{\rho(x')}{\rho(x)} \rho(x) = \omega_{xx'} \rho(x') = \omega_{x'x} \rho(x') = T(x' \rightarrow x)\rho(x'), \quad (1.3)$$

所以其达到了细致平衡, 也就是说系统达到的平衡是 x 数列分布满足 $\rho(x)$ 概率密度的平衡. \square