Chapter 2

Simulated annealing

2.1 Introduction of the algorithm

In its original form [KIR82], [ČER85] the simulated annealing algorithm is based on the analogy between the simulation of the annealing of solids and the problem of solving large combinatorial optimization problems. For this reason the algorithm became known as "simulated annealing". In condensed matter physics, annealing denotes a physical process in which a solid in a *heat bath* is heated up by increasing the temperature of the heat bath to a maximum value at which all particles of the solid randomly arrange themselves in the liquid phase, followed by cooling through slowly lowering the temperature of the heat bath. In this way, all particles arrange themselves in the low energy ground state of a corresponding lattice, provided the maximum temperature is sufficiently high and the cooling is carried out sufficiently slowly. Starting off at the maximum value of the temperature, the cooling phase of the annealing process can be described as follows. At each temperature value T, the solid is allowed to reach *thermal equilibrium*, characterized by a probability of being in a state with energy E given by the *Boltzmann distribution*:

$$Pr\{\mathbf{E} = E\} = \frac{1}{Z(T)} \cdot \exp\left(-\frac{E}{k_B T}\right), \tag{2.1}$$

where $Z(T)$ is a normalization factor, known as the *partition function*, depending on the temperature T and k_B is the *Boltzmann con-*

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stant. The factor $\exp\left(-\frac{E}{k_B T}\right)$ is known as the *Boltzmann factor.* As the temperature decreases, the Boltzmann distribution concentrates on the states with lowest energy and finally, when the temperature approaches zero, only the minimum energy states have a non-zero probability of occurrence. However, it is well known [KIR82] that if the cooling is too rapid, i.e. if the solid is not allowed to reach thermal equilibrium for each temperature value, defects can be 'frozen' into the solid and metastable amorphous structures can be reached rather than the low energy crystalline lattice structure. Furthermore, in a process known in condensed matter physics as *quenching*, the temperature of the heat bath is lowered instantaneously, which results again in a freezing of the particles in the solid into one of the metastable amorphous structures.

To simulate the evolution to thermal equilibrium of a solid for a fixed value of the temperature T, Metropolis *et al.* [MET53] proposed a *Monte Carlo method*, which generates sequences of states of the solid in the following way. Given the current state of the solid, characterized by the positions of its particles, a small, randomly generated, perturbation is applied by a small displacement of a randomly chosen particle. If the difference in energy, ΔE, between the current state and the slightly perturbed one is **negative**, i.e. if the perturbation results in a lower energy for the solid, then the process is continued with the new state. If $\Delta E \geq 0$, then the probability of acceptance of the perturbed state is given by $\exp(-\frac{\Delta E}{k_B T})$. This acceptance rule for new states is referred to as the *Metropolis criterion.* Following this criterion, the system eventually evolves into thermal equilibrium, i.e. after a large number of perturbations, using the aforementioned acceptance criterion, the probability distribution of the states approaches the Boltzmann distribution, given by eq. 2.1. In statistical mechanics this Monte Carlo method, which is known as the *Metropolis algorithm*, is a well-known method used to estimate averages or integrals by means of random sampling techniques; for review articles see e.g. [BAR76], [BIN78], [HAS70] and [WOOD68].

The Metropolis algorithm can also be used to generate sequences of configurations of a combinatorial optimization problem. In that case, the configurations assume the role of the states of a solid while the cost function C and the *control parameter* c take the roles of energy