Statistical Mechanics of an NP-complete Problem: Subset Sum

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Abstract

We study statistical properties of an NP-complete problem, the subset sum, using the methods and concepts of statistical mechanics. The problem is a generalization of the number partitioning problem, which is also an NP-complete problem and has been studied in the physics literature. The asymptotic expressions for the number of solutions are obtained. These results applied to the number partitioning problem as a special case are compared with those which were previously obtained by a different method. We discuss the limit of applicability of the techniques of statistical mechanics to the present problem.

1 Introduction

The methods and concepts of statistical mechanics have turned out to be quite useful in the study of problems in computer science and related fields. In particular, the techniques which have originally been developed in the spin glass theory have been successfully applied to the investigation of the properties of NP-complete problems in the theory of computational complexity [1]. Some of them include the travelling salesman [2], graph partitioning [3], K-SAT [4], knapsack [5], vertex cover [6] and other problems [7, 8]. Roughly speaking, NP-complete problems are a class of problems which are difficult to solve, in the sense that so far no one has succeeded in devising (and in fact it is believed to be

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impossible to design) an algorithm to determine in polynomial time whether or not there is a solution to given input data. NP-complete problems have been extensively studied, but still pose many open questions [1,9].

The issue of primary interest to computer scientists is to find an algorithm which efficiently finds a solution to given input data, for which purpose statistical mechanics may not be of direct use because the latter is suitable to reveal typical properties of many-body systems. Recently, however, statistical properties of these problems have been receiving increasing attention since it has gradually been recognized that a generally hard problem can sometimes be solved relatively easily under certain criteria with the assistance of statistical mechanics ideas [10].

For a wide class of NP-complete problems, the following situation happens. A problem has a parameter and, when the size of the problem becomes large, there appears a "critical" value of the parameter such that below it an algorithm can efficiently find a solution (easy region) but above it the same algorithm no longer works effectively (hard region). This happens because the definition of NP-completeness is based on the *worst* case analysis. A problem can be classified as a difficult one if there are only a few difficult instances. The sudden change of the statistical properties of a problem is in many respects similar to a phase transition, a concept from statistical mechanics. In fact, the methods for studying phase transitions have turned out to be powerful tools to understand the properties of the above-mentioned phenomena. These observations suggest that the *typical* case study will play increasingly important roles in computer science and accordingly the methods from statistical mechanics will provide useful tools.

In typical case studies, one usually considers a randomized version of a problem. In other words, our main interest is in the properties of the problem averaged over possible realizations of input data. The randomized problems share many features with spin glass systems and have been often studied using the techniques of the spin glass theory. In particular the replica method has allowed us to analyze the problems, many of which would have been impossible to deal with without it. Nonetheless the resulting saddle point analysis, known as the problem of replica-symmetry breaking, is often so hard that it is usually difficult to get complete understanding of the problem. Hence, to gain more insights, it is important to study problems which are solvable without using replicas.

The number partitioning problem seems to be an ideal example from this point of view [11–14]. Suppose that one is given a set of positive integers $\mathcal{A} = \{a_1, a_2, \ldots, a_N\}$ and asked to divide this into two subsets with the same value of the sums. In other words, one tries to find a subset $\mathcal{A}' \subset \mathcal{A}$ which minimizes the partition difference

$$\left| \sum_{\mathcal{A}'} a_j - \sum_{\mathcal{A}\backslash\mathcal{A}'} a_j \right| . \tag{1.1}$$

A subset $\mathcal{A}'$ with zero partition difference is called a perfect partition, whereas a subset with a positive partition difference is termed an imperfect partition. It has been argued that this problem shows a sharp change of states, reminiscent of a phase transition, between easy and hard regions [12–15]. In addition, the problem has a lot of practical applications such as multiprocessor scheduling and minimization of VLSI circuit size.

The analysis in [13,14] starts from taking the partition difference to be the Hamiltonian. Then a perfect partition corresponds to a ground state of the Hamiltonian and an imperfect partition to a configuration with positive energy. By applying the statistical mechanics methods and a saddle point approximation in the large-N limit, several results have been obtained without using replicas. The phase transition behaviour of the problem, found numerically [15], was understandable through those results. But the expressions obtained in his analysis show peculiar high temperature behaviours as will be shown below. In particular, the partition function does not give the correct entropy in the limit of high temperature. Hence his results are not expected to give reliable predictions for imperfect partitions.

The main purpose of this paper is to propose an alternative approach to the number partitioning problem applicable to imperfect partitions as well. We study a generalized version of the number partitioning problem: the subset sum [1]. By using some basic concepts and methods of statistical mechanics, the asymptotic expressions of the number of solutions are obtained. Our results specialized to the number partitioning problem are compared with the previously obtained predictions. It is shown that our results are applicable to the cases where the predictions of the previous analysis do not agree with an exactly solvable example. Our discussions are mainly restricted to the easy region although the hard region could also be considered by similar arguments using the ideas in [16].

The rest of the paper is organized as follows. In the next section, we introduce the subset sum and reformulate it in terms of a Hamiltonian. By using the canonical ensemble, the asymptotic number of solutions is estimated in section 3. Based on the results, we discuss a crossover between easy and hard regions of the subset sum in section 4. In section 5, the analysis is generalized to the case with constraint. In section 6, we apply the results to the number partitioning problem and compare the results with those in [13]. Conclusion is given in the last section.

2 Subset Sum

Let us denote $\mathbb{N}_+ = \{1, 2, \cdots\}$, the set of positive integers. The subset sum is an example of NP-complete problems in which one asks, for a given set of $\mathcal{A} = \{a_1, a_2, \cdots, a_N\}$ with $a_j \in \mathbb{N}_+$ $(j = 1, 2, \cdots, N)$ and $E \in \mathbb{N}_+$, whether or not there exists a subset $\mathcal{A}' \subset A$ such that the sum of the elements of $\mathcal{A}'$ is E [1]. To formulate the problem, we introduce a Hamiltonian (or energy)

$$H = \sum_{j=1}^{N} a_j n_j, \tag{2.1}$$

where $n_j \in \{0, 1\}$ $(j = 1, 2, \cdots, N)$, and the subset sum is equivalent to asking whether or not there exists a configuration $\{n_1, n_2, \cdots, n_N\}$ such that $H = E$. A configuration which satisfies $H = E$ is called a solution in the following.

There are several versions of the problem. The original one is the decision problem; one only asks whether there exists a solution or not. Once one learns that the answer to the decision problem is yes, however, it would be quite natural next to ask how many solutions there are. This is called the counting (or enumeration) version of the problem. On the other hand, if there is no solution, one might try to find the best possible configuration which minimizes the energy difference from the given E. This is the optimization version of the problem. Of course these versions are closely related to each other. In the following treatments, we focus on the counting version of the problem, for which statistical mechanics provide powerful analytical tools. The number of solutions for a given energy E will be denoted by $W(E)$.

3 Statistical Mechanical Analysis of Subset Sum

Evaluation of the exact value of $W(E)$ for given $\mathcal{A}$ and E is still a question of complicated combinatorics and is very hard. In particular, fixing the value of E is a very strong constraint which renders the counting almost intractable. In the terminology of statistical mechanics, considering the problem with a fixed value of E corresponds to working in the microcanonical ensemble. For many purposes in practice, however, one is interested in the asymptotic behaviours for a large N and is satisfied with approximate expressions of $W(E)$; an exact expression of $W(E)$ is unnecessary and can even obscure the essential aspects of the problem. The experience in the study of statistical mechanics tells us that, in order to know the asymptotic behaviour of $W(E)$, it is much easier to work in the canonical ensemble. This is a superposition of the microcanonical ensembles for all possible values of the energy with the Boltzmann factor $e^{-\beta E}$, where β is the inverse temperature. In this section, the set $\mathcal{A}$ is still fixed; statistics over many $\mathcal{A}$ is not considered.

Simplicity of the analysis of the subset sum compared with other problems stems from a compact expression for the partition function. For a given $\mathcal{A}$, the partition function Z is simply given by

$$\begin{aligned} Z = \sum_{\{n_j\}} e^{-\beta H} &= \sum_{n_1=0,1} \sum_{n_2=0,1} \cdots \sum_{n_N=0,1} e^{-\beta H} \\ &= (1+e^{-\beta a_1})(1+e^{-\beta a_2}) \cdots (1+e^{-\beta a_N}). \end{aligned} \tag{3.1}$$

From this one can calculate the average values of various physical quantities. The average here means the thermal average and is denoted by $\langle \cdots \rangle$. The average energy $\langle E \rangle$ for a given value of β is given by

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z = \sum_{j=1}^{N} \frac{a_j}{1+e^{\beta a_j}}. \tag{3.2}$$

Note that the value of $\langle E \rangle$ can be controlled by changing β. As β is increased from $-\infty$ to ∞, the average energy $\langle E \rangle$ decreases from $\sum_{j=1}^{N} a_j$ to 0. In usual statistical mechanics, the temperature and hence β should be positive. For our present problem, however, the temperature is introduced only as a parameter to control the average energy. A negative value of β is also allowed in our problem. The fluctuation of the energy is similarly calculated as

$$\langle (E - \langle E \rangle)^2 \rangle = \frac{\partial^2}{\partial \beta^2} \log Z = \sum_{j=1}^{N} \frac{a_j^2}{(1 + e^{\beta a_j})(1 + e^{-\beta a_j})}. \tag{3.3}$$

Here we go back to (3.1) and observe that $W(E)$, the number of solutions to the condition $H = E$, appears as the coefficient of the Eth power of q $(= e^{-\beta})$ in Z; the expansion of Z in terms of q gives

$$Z = \sum_{E=0}^{E_{\max}} W(E)\, q^E \tag{3.4}$$

with $E_{\max} = a_1 + a_2 + \cdots + a_N$. Moreover, since Z is a polynomial in q, (3.4) can be inverted easily: $W(E)$ has an integral representation

$$W(E) = \int_C \frac{dq}{2\pi i} Z q^{-E-1} \tag{3.5}$$

with C being a contour enclosing the origin anticlockwise on the complex q plane. It is important to notice that the contour C in (3.5) can be deformed arbitrarily as far as it encloses the origin anticlockwise.

Now we consider the asymptotics of $W(E)$ as $N \to \infty$. One should specify how this limit is taken since changing N also implies changing $\mathcal{A}$ simultaneously. To avoid this difficulty, let us suppose for the moment that one first has an infinite set $\mathcal{A}_\infty = \{a_1, a_2, \cdots\}$, each element of which is taken from a finite set of $\{1, 2, \cdots, L\}$, with $L \in \mathbb{N}_+$. Then the set $\mathcal{A}$ can be regarded as a collection of the first N elements of $\mathcal{A}_\infty$. The limit $N \to \infty$ is defined without ambiguities in this way.

Since a_j satisfies $1 \le a_j \le L$ for all j, a simple estimation of (3.3) shows that the fluctuation of the energy is of order N when β is finite. Hence the fluctuation of the energy per system size N, i.e., $\langle (E/N - \langle E \rangle/N)^2 \rangle$, tends to zero as $N \to \infty$. Let β_0 be the value of β such that the average energy $\langle E \rangle$ is equal to E. Then one takes the contour C in (3.5) to be a circle with radius $e^{-\beta_0}$ and uses the phase variable θ defined by $q = e^{-\beta_0 + i\theta}$ to find

$$W(E) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta e^{\log Z + \beta_0 E - iE\theta}. \tag{3.6}$$

It is not difficult to verify that the saddle point of this integrand is at $\theta = 0$. (When the g.c.d. of $\mathcal{A}$ is not one, there appear other saddle points with the same order of contributions. But, when N is large enough, it is almost sure that the g.c.d. of $\mathcal{A}$ is one, which we assume in what follows.)

The quantities in the exponent on the right hand side of (3.6) are all of order N. Therefore we can use the method of steepest descent to evaluate the asymptotic behaviour of the integral. Expanding $\log Z$ around $\beta = \beta_0$ to second order leads to

$$W(E) = e^{\log Z|_{\beta=\beta_0} + \beta_0 E} \cdot \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp\left(-\frac{\theta^2}{2} \frac{\partial^2}{\partial \beta^2} \log Z|_{\beta=\beta_0} \right). \tag{3.7}$$

Since the second derivative of $\log Z$ is the fluctuation of the energy (3.3) and is of order N, the integration range may be extended to $\pm\infty$. The result is

$$W(E) \approx \frac{\exp\left[\log Z|_{\beta=\beta_0} + \beta_0 E\right]}{\sqrt{2\pi \frac{\partial^2}{\partial \beta^2} \log Z|_{\beta=\beta_0}}}. \tag{3.8}$$

Here and in the following the symbol $\approx$ means that the ratio of the right and left hand sides tends to unity as $N \to \infty$. After rewriting β_0 back to β, we finally obtain the asymptotic expression of $W(E)$ for a given value of E via a common parameter β as

$$W(E) \approx \frac{\exp\left[\sum_{j=1}^{N} \log(1 + e^{-\beta a_j}) + \beta \sum_{j=1}^{N} a_j/(1 + e^{\beta a_j})\right]}{\sqrt{2\pi \sum_{j=1}^{N} a_j^2/(1 + e^{\beta a_j})(1 + e^{-\beta a_j})}}, \tag{3.9}$$

$$E = \sum_{j=1}^{N} \frac{a_j}{1 + e^{\beta a_j}}. \tag{3.10}$$

A numerical check of (3.9) and (3.10) is shown in Fig. 1. As far as one sees on this scale, the agreement of our predictions and simulational data is satisfactory for the entire range of the energy.

One may notice that the obtained expressions, (3.9) and (3.10), do not depend on L. This is plausible since the number of solutions depends only on the elements of $\mathcal{A}$, not directly on the set from which elements of $\mathcal{A}$ have been taken. One should remember in this relation that the validity of the saddle point analysis depends on L. The expressions, (3.9) and (3.10), become better approximations as $N \to \infty$ for a fixed value of L. It would not be surprising if the expressions do not agree very well with simulational data when L is sufficiently large so that $W(E)$ is of $O(1)$. In particular one should not use (3.9) in the parameter region which gives $W(E) < 1$ as will be discussed below.

4 Easy/Hard Regions

Numerical simulations in [15] suggest that there exist easy and hard regions for a randomized version of the subset sum, in which one considers statistics over many samples of $\mathcal{A}$ with each a_j drawn from $\{1, 2, \ldots, L\}$ uniformly. In simulations, one checks if there exists a solution for many samples of $\mathcal{A}$ with given N, L and E. Then for each N and E, one plots the probability that there is at least one solution as a function of $\kappa = \log_2 L/N$. Then it is observed that the probability decreases fairly sharply from 1 to 0 as κ increases from zero to ∞. As N becomes larger, the decrease of the probability occurs in a narrower range of κ. In fact, the system appears to have a sharp transition at a critical value κ_c in the limit of $N, L \to \infty$ [15]. In this section, we estimate the critical value κ_c of the randomized subset sum by using the results of the last section.

The analysis in the last section gives us the asymptotic formula for a fixed $\mathcal{A}$. To apply the results to the randomized version of the problem, one has to notice that, as N becomes large, the sample dependence of (3.9) and (3.10) is suppressed increasingly. In fact, in the limit $N \to \infty$ with L fixed, there would be no sample dependence so that the average properties of these quantities coincide with those of a typical sample. To see this, let us define the density of $y_j = a_j/L$ $(1 \le j \le N)$ to be $\rho_N(y) = \frac{1}{N}\sum_{j=1}^{N}\delta(y - y_j)$. Since we draw the a_j uniformly, we have $\lim_{N\to\infty} \rho_N(y) = \rho(y)$ where $\rho(y) = 1$ for $0 \le y \le 1$ and $\rho(y) = 0$ otherwise. In addition, in this limit, summations in (3.9) and (3.10) are replaced by integrals, resulting in

$$W(E) \approx \frac{\exp\left[N\int_0^1 dy\,\{\log(1+e^{-\alpha y}) + \alpha y/(1+e^{\alpha y})\}\right]}{\sqrt{2\pi N L^2 \int_0^1 dy y^2/(1+e^{\alpha y})(1+e^{-\alpha y})}}, \tag{4.1}$$

$$x = \frac{E}{N\cdot L} \approx \int_0^1 dy \frac{y}{1+e^{\alpha y}}, \tag{4.2}$$

where we have introduced a scaled inverse temperature $\alpha = \beta/L$. The parameter α controls x, the energy divided by $N \cdot L$; as α is increased from $-\infty$ to ∞, x decreases from 1/2 to 0. The validity of these expressions is determined only by the values of N and L. For a given N, they are valid for sufficiently small L. Even though L changes, however, these expressions are expected to be good approximations as long as N is relatively large or when κ is fairly smaller than κ_c. On the other hand, the reliability of these expressions is unclear for $\kappa \gg \kappa_c$. In fact, there is evidence that the average minimal cost is not self-averaging in this region [12]. The value of κ below which the above formulas are valid increases as N and L increase, and finally it reaches κ_c in the limit $N, L \to \infty$. It is important to notice that the value of κ_c can be determined by the condition $W(E) = 1$ in the limit $N, L \to \infty$ because $W(E)$ is the expectation value of the number of configurations. We therefore find

$$\kappa_c = \frac{1}{\log 2}\int_0^1 dy \left[\log(1+e^{-\alpha y}) + \frac{\alpha y}{1+e^{\alpha y}}\right] \tag{4.3}$$

with α determined by (4.2) for a given value of x. For $\kappa < \kappa_c$, exponentially many solutions are expected to exist and one of them can be found fairly easily. On the other hand, for $\kappa > \kappa_c$, there is practically no solution and hence it is virtually impossible to find one. The easy/hard regions of the randomized subset sum are shown in Fig. 2.

5 Constrained Case

In some applications, one might encounter a situation where the number of a_j's is given. In this section, our previous analysis is generalized to the *constrained* case where the number of chosen a_j's is fixed to M. Instead of considering directly the system with constraint, we again take a superposition of the problems with various values of M. In the language of statistical mechanics, we work in the grand canonical ensemble. Let us define a Hamiltonian

$$H_{\rm c} = \sum_{j=1}^{N} a_j n_j - \frac{\mu}{\beta} \sum_{j=1}^{N} n_j. \tag{5.1}$$

The first term is nothing but the Hamiltonian (2.1) for the unconstrained subset sum. The second term is introduced to control the number of a_j's by changing the parameter μ, the chemical potential. The grand partition function is evaluated as

$$\begin{aligned} \Theta &= \sum_{\{n_j\}} e^{-\beta H_{\rm c}} \\ &= (1 + e^{\mu} e^{-\beta a_1})(1 + e^{\mu} e^{-\beta a_2}) \cdots (1 + e^{\mu} e^{-\beta a_N}) \\ &= \sum_{M=0}^{N} \sum_{E=0}^{E_{\max}} W(M, E) e^{\mu M} e^{-\beta E}, \end{aligned} \tag{5.2}$$

with $E_{\max} = a_1 + a_2 + \cdots + a_N$ as before. Here $W(M, E)$ is the number of configurations which satisfy $\sum_{j=1}^{N} a_j n_j = E$ and $\sum_{j=1}^{N} n_j = M$ simultaneously.

For given values of μ and β, the average number, energy and second moments of these quantities are expressed as

$$\langle M \rangle = \frac{\partial}{\partial \mu} \log \Theta = \sum_{j=1}^{N} \frac{1}{1 + e^{\beta a_j - \mu}}, \tag{5.3}$$

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log \Theta = \sum_{j=1}^{N} \frac{a_j}{1 + e^{\beta a_j - \mu}}, \tag{5.4}$$

$$\langle (M - \langle M \rangle)^2 \rangle = \frac{\partial^2}{\partial \mu^2} \log \Theta = \sum_{j=1}^{N} \frac{1}{(1 + e^{\beta a_j - \mu})(1 + e^{-\beta a_j + \mu})}, \tag{5.5}$$

$$\langle (M - \langle M \rangle)(E - \langle E \rangle) \rangle = -\frac{\partial^2}{\partial \beta \partial \mu} \log \Theta = \sum_{j=1}^{N} \frac{a_j}{(1 + e^{\beta a_j - \mu})(1 + e^{-\beta a_j + \mu})}, \tag{5.6}$$

$$\langle (E - \langle E \rangle)^2 \rangle = \frac{\partial^2}{\partial \beta^2} \log \Theta = \sum_{j=1}^{N} \frac{a_j^2}{(1 + e^{\beta a_j - \mu})(1 + e^{-\beta a_j + \mu})}. \tag{5.7}$$

Similarly to the unconstrained case, one can show that the fluctuations of the number and energy divided by the system size vanish as $N \to \infty$ so that one can apply the saddle point method. The resulting asymptotic expression for $W(M,E)$ reads

$$W(M,E) \approx \frac{\exp[\log\Theta + \beta E - \mu M]}{2\pi\sqrt{D}} \tag{5.8}$$

with D being

$$D = \begin{vmatrix} \frac{\partial^2}{\partial\mu^2}\log\Theta & -\frac{\partial^2}{\partial\beta\partial\mu}\log\Theta \\ -\frac{\partial^2}{\partial\beta\partial\mu}\log\Theta & \frac{\partial^2}{\partial\beta^2}\log\Theta. \end{vmatrix} \tag{5.9}$$

The values of M and E are given by (5.3) and (5.4), respectively. Using these expressions, one can discuss the easy/hard regions of the constrained subset sum. The analysis is almost the same as that in the last section and is omitted here.

6 Number Partitioning Problem

As already mentioned in the introduction, the subset sum is regarded as a generalization of the number partitioning problem. In this section, we apply our previous discussions to the number partitioning problem. Our results are compared with those in [13, 14], which are briefly reviewed in Appendix A with some remarks.

Let us first establish an explicit relationship between the subset sum and the number partitioning problem. If one introduces the spin variables by

$$s_j = 2n_j - 1, \tag{6.1}$$

it is not difficult to see

$$\tilde{H} := \left| 2H - \sum_{j=1}^{N} a_j \right| = \left| \sum_{j=1}^{N} a_j s_j \right|. \tag{6.2}$$

This is exactly the Hamiltonian of the number partitioning problem studied in [13, 14].

The number of solutions of $\tilde{H} = \tilde{E}$, which we denote by $\tilde{W}(\tilde{E})$, is related to $W(E)$ by

$$\tilde{W}(\tilde{E}) = \begin{cases} W(\frac{1}{2}\sum_{j=1}^{N} a_j) & (\tilde{E} = 0) \\ W(\frac{1}{2}\tilde{E} + \frac{1}{2}\sum_{j=1}^{N} a_j) + W(-\frac{1}{2}\tilde{E} + \frac{1}{2}\sum_{j=1}^{N} a_j) & (\tilde{E} > 0) \end{cases}. \tag{6.3}$$

Of special interest is the case of $\tilde{E} = 0$, a solution of which is called a perfect solution in the number partitioning problem. In the subset sum, this corresponds to the energy $E = \frac{1}{2}\sum_{j=1}^{N} a_j$. Clearly there is no perfect solutions if $\sum_{j=1}^{N} a_j$ is odd; we assume $\sum_{j=1}^{N} a_j$ is even in the following. In terms of β, considering perfect solutions corresponds to $\beta = 0$ from (3.10). Setting $\beta = 0$ in (3.9) leads to

$$\tilde{W}(0) \approx \frac{2^N}{\sqrt{\frac{\pi}{2}\sum_{j=1}^{N} a_j^2}}, \tag{6.4}$$

which is expected to be the number of perfect solutions to the number partitioning problem. In fact (6.4) agrees with the previously obtained result in [13, 14]. Hence, as far as the number of perfect solutions for the number partitioning problem is concerned, our method gives exactly the same answer as in [13, 14].

The difference between our formula and that in [13, 14] becomes manifest for a finite value of $\tilde{E}$. We demonstrate this by considering the number partitioning problem for a special case where $a_1 = a_2 = \cdots = a_N = 1$ with N even. In this case, the Hamiltonian reads $\tilde{H} = |\sum_{j=1}^{N} s_j|$, and it is possible to write down the partition function $\tilde{Z} = \sum_{\{s_j\}} e^{-\beta\tilde{H}}$ explicitly:

$$\begin{aligned}\tilde{Z} &= \sum_{j=1}^{N} \binom{N}{j} e^{-\beta|N-2j|} \\ &= \binom{N}{\frac{N}{2}} + 2\sum_{j=1}^{N/2} \binom{N}{\frac{N}{2}+j} e^{-2\beta j}.\end{aligned} \tag{6.5}$$

This formula indicates that there are solutions for even $\tilde{E}$ and that $\tilde{W}(\tilde{E})$ is

$$\tilde{W}(\tilde{E}) = \begin{cases} \binom{N}{N/2} \approx \dfrac{2^N}{\sqrt{\frac{\pi}{2}N}} & (\tilde{E}=0) \\ 2\binom{N}{N/2+j} \approx \dfrac{2\exp N\left[-(\frac{1}{2}-\frac{j}{N})\log(\frac{1}{2}-\frac{j}{N}) - (\frac{1}{2}+\frac{j}{N})\log(\frac{1}{2}+\frac{j}{N})\right]}{\sqrt{2\pi N(\frac{1}{2}+\frac{j}{N})(\frac{1}{2}-\frac{j}{N})}} & (\tilde{E}=2j) \end{cases}, \tag{6.6}$$

where the asymptotics are also indicated. For the present case with $a_j = 1$ $(1 \le j \le N)$, (3.10) is simply reverted as $\beta = \log(N/E - 1)$. Then, using Stirling's formula, one can confirm that our formula (3.9) gives correct asymptotics in (6.6) for the entire range of energy. By contrast the partition function in [13,14], which we denote by $\tilde{Z}'$, for the present case can be written as

$$\tilde{Z}' = \frac{2^N}{\sqrt{\frac{\pi}{2}N}} \left(1 + 2\sum_{j=1}^{\infty} e^{-2\beta j}\right). \tag{6.7}$$

This indicates that there are solutions for even $\tilde{E}$ and that $\tilde{W}(\tilde{E})$ is asymptotically $2^N/\sqrt{\frac{\pi}{2}N}$ for $\tilde{E} = 0$ and $2^{N+1}/\sqrt{\frac{\pi}{2}N}$ for $\tilde{E} = 2j$. As is clear from (6.6), the correct asymptotics is predicted only for $\tilde{E} = 0$. One may notice that the arguments in [13, 14] are somewhat different from ours. There, the energy $\tilde{E}$ and the entropy $\tilde{S}$ are calculated from the partition function (6.7), following the usual prescriptions of statistical mechanics. It is assumed that $\exp(\tilde{S})$ gives the number of solutions. The obtained expressions again do not give the correct asymptotics of $\tilde{W}(\tilde{E})$ when $\tilde{E} > 0$. Our conclusion is that the results of [13, 14] give the correct asymptotic value for $\tilde{E} = 0$ but not for $\tilde{E} > 0$.

The reason for this difficulty is traced back to the application of statistical mechanics techniques to the system for which the number of solutions of $\tilde{H} = \tilde{E}$ decreases as $\tilde{E}$ increases. It can be seen from Fig. 1 that the number partitioning problem is indeed an example with this anomalous property if one notes that $\tilde{E} = 0$ corresponds to the peak of the curve. The problem is that, for such systems, usual prescriptions of the canonical ensemble do not work. For normal physical systems, the number of states $W(E)$ increases as a function of the energy E. The number of states multiplied by the Boltzmann factor $W(E)e^{-\beta E}$ takes a maximum at some value of E. The peak around this point becomes drastically sharp as the system size increases. Then the equivalence of microcanonical and canonical ensembles holds so that we can study the thermodynamic behaviours of the system in either ensemble. For systems with decreasing $W(E)$, however, $W(E)e^{-\beta E}$ is a monotone decreasing function. The fluctuation of the energy does not tend to zero even when the system size increases indefinitely, and consequently one can not control the energy by changing the temperature. As a result, the equivalence of ensembles does not hold. The exponential of the entropy calculated in the canonical ensemble and the coefficient of the expansion of Z in powers of $e^{-\beta E}$ do not agree even in the thermodynamic limit; in addition, neither of these quantities give the correct asymptotics of the number of configurations $W(E)$. This problem may be overcome by considering a negative temperature as we did for the subset sum, but a direct analysis of the number partitioning problem described by (6.2) would then be much more difficult.

Before closing this section, we discuss the randomized number partitioning problem with a constraint in which one asks whether or not there exists a perfect solution with $\sum_{j=1}^{N} s_j$ fixed. In the language of subset sum, this corresponds to fixing M since $\sum_{j=1}^{N} s_j = \sum_{j=1}^{N}(2n_j - 1) = 2M - N$. In [12, 14], it has been found that there is a phase transition in the limit $M, N \to \infty$ with $m = 2M/N - 1$ fixed. We can reproduce this phenomenon from the results of section 5. In the limit N, L and $M \to \infty$, summations in (5.3) and (5.4) are replaced by integrals. They are written as, for a uniform distribution,

$$\frac{1}{2}(1+m) = \int_0^1 dy \frac{1}{1+e^{\alpha y - \mu}} = 1 - \frac{1}{\alpha} \log \frac{e^{\alpha} + e^{\mu}}{1 + e^{\mu}}, \tag{6.8}$$

$$x = \int_0^1 dy \frac{y}{1+e^{\alpha y - \mu}}, \tag{6.9}$$

where $\alpha = \beta/L$ and $x = E/N \cdot L$ as before. Since (6.8) is easily reverted as

$$\mu = \log \frac{e^{\alpha} - e^{\alpha(1-m)/2}}{e^{\alpha(1-m)/2} - 1}, \tag{6.10}$$

one can regard x as a function of α and m. Then, for a fixed m ($-1 \le m \le 1$), one sees that x decreases from $(1+m)(3-m)/8$ to $(1+m)^2/8$ as α is increased from $-\infty$ to ∞. There are few or no configurations for energy corresponding to x outside this range. If we note that the perfect solution corresponds to $x = 1/4$, we find that there are extensive number of perfect solutions when $|m| < \sqrt{2} - 1$ and there is practically no perfect solution when $|m| > \sqrt{2} - 1$. Hence we conclude that there is a phase transition at $m_c = \sqrt{2} - 1$, in agreement with the previous analysis [12, 14].

7 Conclusion

We have studied the statistical properties of the subset sum, which is a generalization of the number partitioning problem. The basic ideas and methods of statistical mechanics enabled us to study the asymptotic behaviour of the number of solutions for a given set of input data. The expressions (3.9) and (3.10) represent the main results of this paper. The agreement of the predictions with simulational data have been found satisfactory. Our results have been compared with those which were previously obtained by a different method. They agreed with each other for the number of perfect solutions of the number partitioning problem. On the other hand, in the case of the subset sum, only our analysis gave the correct asymptotics over the entire range of energy. The reason why the validity of the results in [13,14] is restricted to perfect solutions has been argued to be that the entropy calculated in canonical ensemble does not necessarily give the logarithm of the number of configurations for systems with a decreasing number of states as the energy increases. In such anomalous systems, one should be extremely careful in using the equivalence between microcanonical, canonical, and grand canonical ensembles.

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Appendix A Some Remarks on the Analysis in [13, 14]

In this Appendix, we briefly review the results in [13, 14] and give a few remarks on the analysis. Our notations are slightly different from the original ones for consistency with the main text. The g.c.d. of $\mathcal{A}$ is assumed to be unity in the following. After some manipulations, the partition function $\tilde{Z}$ for the Hamiltonian (6.2) is rewritten as

$$\tilde{Z} = \sum_{\{s_j\}} e^{-\beta \tilde{H}} = 2^N \int_{-\pi/2}^{\pi/2} \frac{dy}{\pi} e^{NG(y)}, \tag{A.1}$$

where $\beta(\geq 0)$ is the inverse temperature and

$$G(y) = \frac{1}{N} \sum_{j=1}^{N} \log \cos(\beta a_j \tan y). \tag{A.2}$$

Then it has been argued that, for a large N, the integral in (A.1) can be evaluated using the Laplace method. There exist an infinite number of points which give the maximum value of $\mathrm{Re}\{G(y)\}$. The main contributions are expected to come from the points

$$y_k = \arctan\left(\frac{\pi}{\beta} k\right), \quad k = 0, \pm 1, \pm 2, \ldots. \tag{A.3}$$

It is not difficult to confirm $\mathrm{Re}\{G(y)\} \leq 0$ for general y and $\mathrm{Re}\{G(y_k)\} = G'(y_k) = 0$ and $G''(y_k) < 0$, so that y_k's of (A.3) certainly give the maximum of $\mathrm{Re}\{G(y)\}$. The contributions from these y_k's can be summed up explicitly, and the result is

$$\begin{aligned}
\tilde{Z} &\approx 2^N \sum_{k=-\infty}^{\infty} e^{NG(y_k)} \int_{-\infty}^{\infty} \frac{dy}{\pi} e^{\frac{N}{2}G''(y_k)y^2} \\
&= \frac{2^N}{\beta\sqrt{\frac{\pi}{2}\sum_{j=1}^N {a_j}^2}} \sum_{k=-\infty}^{\infty} \frac{(-1)^{k\lambda}}{1+(\frac{\pi}{\beta}k)^2} \\
&= \begin{cases} \frac{2^N}{\sqrt{\frac{\pi}{2}\sum_{j=1}^N {a_j}^2}} \coth\beta & (\lambda : \text{even}) \\ \frac{2^N}{\sqrt{\frac{\pi}{2}\sum_{j=1}^N {a_j}^2}} \mathrm{cosech}\beta & (\lambda : \text{odd}) \end{cases},
\end{aligned} \tag{A.4}$$

where $\lambda = \sum_{j=1}^N a_j$. Here we remark that in [13, 14] the formula for the case of odd λ is missing. (Also, in the arguments of the constrained case in [14], the results are presented only for the case of even N, but one has to consider the case of odd N separately.) Nevertheless, we only consider the case where λ is even in the following, because the odd λ case can be discussed similarly.

One notes that the expression (A.4) diverges as $\beta \to 0$ while the correct limiting value is clearly 2^N from the definition (A.1). Hence, as mentioned in the main text, his result (A.4) is not valid at least for small β (or large T).

In [13, 14], the hard region was also discussed using (A.4). In particular, the average minimum cost was estimated. One should use the finite-temperature expression of the partition function (A.4) to analyze the non-vanishing value of average minimum cost in the hard region. However, since (A.4) is not reliable for large T, the formulas given in [13, 14] should be taken with special caution. The principal source of trouble is in the anomalous properties of the systems with the decreasing number of configurations as the energy increases. There is another point of problems in his analysis as we discuss in the following.

A sign of difficulty is seen from the negative value of the entropy in the hard region. The entropy calculated from the partition function (A.4) reads

$$\tilde{S} = \log \frac{2^N}{\sqrt{\frac{\pi}{2}\sum_{j=1}^N {a_j}^2}} \coth\beta + \frac{\beta}{\sinh\beta \cdot \cosh\beta}. \tag{A.5}$$

The ground state entropy $\tilde{S}_0 = \lim_{\beta\to\infty} \tilde{S}$ is found to be

$$\tilde{S}_0 = \{N - N_c(\mathcal{A})\} \log 2, \tag{A.6}$$

with

$$N_c(\mathcal{A}) = \frac{1}{2} \log_2 \frac{\pi}{2} \sum_{j=1}^N {a_j}^2. \tag{A.7}$$

This is equivalent to (6.4). One notices that, when $N < N_c(\mathcal{A})$, the ground state entropy is negative. In [13, 14], the easy (resp. hard) region is characterized by a positive $\tilde{S}_0$ (resp. a negative $\tilde{S}_0$), i.e., by $N > N_c(\mathcal{A})$ (resp. $N < N_c(\mathcal{A})$). In an appropriate limit, this coincides with $\kappa < \kappa_c$ (resp. $\kappa > \kappa_c$). To avoid the difficulty of negative entropy in the hard region, the author of [13, 14] proposed not to take the $\beta \to \infty$ limit but to use (A.4) only down to the temperature where $\tilde{S} \geq \log 2$. This is an arbitrary process which would not be necessary if we use the exact expression of the entropy.

To identify the problem within his formalism, let us remember that (A.4) was obtained by summing up only the contributions from around extreme points $\{y_k\}$ of (A.3). In the easy region ($N \gg N_c(\mathcal{A})$) the peaks around these points are very sharp and hence the Laplace method gives a good approximation. On the other hand, in the hard region ($N \ll N_c(\mathcal{A})$), there appear a large number of other local maxima, with values not so far from zero and at points located fairly close to the points $\{y_k\}$ of (A.3). One will be easily convinced that this happens by checking a very simple example of $N = 2$. In this case $G(y)$ reads

$$G(y) = \frac{1}{2} \log \cos(\beta a_1 \tan y) + \frac{1}{2} \log \cos(\beta a_2 \tan y), \tag{A.8}$$

where $a_1, a_2 (a_1 < a_2)$ are coprime natural numbers with a_2 sufficiently large corresponding to the hard region.

Figure Captions

Fig. 1: The number of solutions $W(E)$ as a function of the energy E for an example with $N = 20, L = 256$, and $\mathcal{A} = \{218, 13, 227, 193, 70, 134, 89, 198, 205, 147, 227, 190, 27, 239, 192, 131\}$. The theoretical prediction is indistinguishable from the numerical results plotted in dots.

Fig. 2: The easy/hard regions of the randomized subset sum.

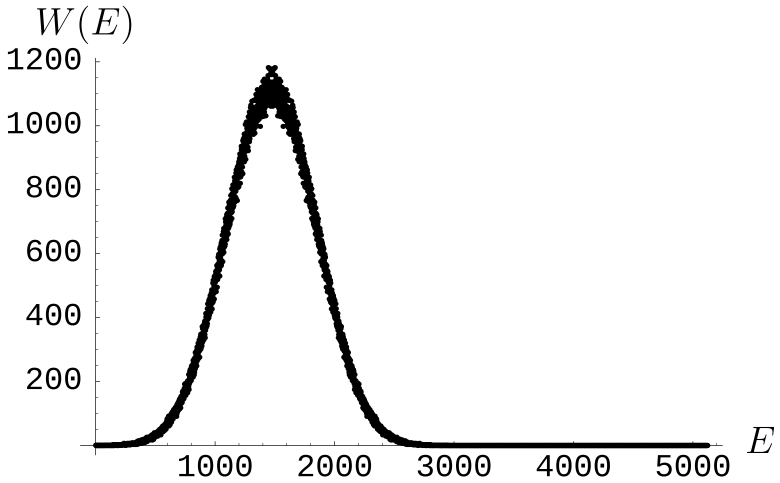

Figure 1

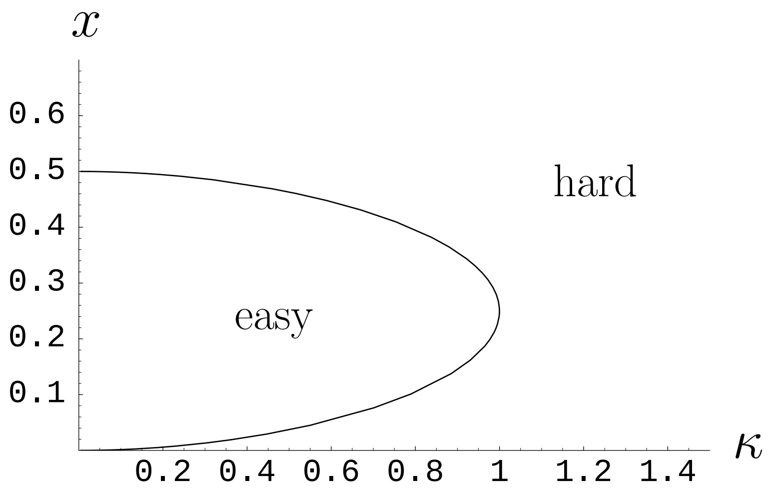

Figure 2