Adiabatic quantum computing solution of the knapsack problem

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(Received

2017)

January 17, 2017

Abstract

We illustrate the adiabatic quantum computing solution of the knapsack problem with both integer profits and weights. For problems with n objects (or items) and integer capacity c, we give specific examples using both an Ising class problem Hamiltonian requiring n+c qubits and a much more efficient one using $n+[\log_2 c]+1$ qubits. The discussion includes a brief mention of classical algorithms for knapsack, applications of this commonly occurring problem, and the relevance of further studies both theoretically and numerically of the behavior of the energy gap. Included too is a demonstration and commentary on a version of quantum search using a certain Ising model. Furthermore, an Appendix presents analytic results concerning the boundary for the easy-versus-hard problem-instance phase transition for the special case subset sum problem.

Key words and phrases

adiabatic quantum computing, knapsack with integer weights, spectral gap, binary variable, Ising Hamiltonian, subset sum, phase transition, quantum search

Introduction

Adiabatic quantum computing (AQC) is an approach (polynomially) equivalent to the circuit model of quantum computing [1]. It has the attraction of being suitable for problems of the combinatorial optimization sort including partitioning, covering, traversing trees and graphs, and logical satisfiability. In fact, early important papers in this field were concerned with the latter topic [2, 3]. This paper concentrates on the AQC solution of the knapsack apportioning problem, but we also remark on such solution of other problems.

Within the AQC method, the ground state of a problem Hamiltonian encodes the solution of interest. The hardware solution arises from the slow-enough evolution of the ground state of an initial simpler Hamiltonian to that of the problem Hamiltonian. Then the problem solution may be read out. Without going in to further detail, the required evolution time is dictated by the inverse square of the spectral gap, the minimum energy difference between the ground and first excited states. Traditionally the adiabatic theorem has been based upon time-dependent perturbation theory, and of course more recently there is a variety of more specific and rigorous results. Experimentally, so far AQC has been demonstrated in NMR (nuclear magnetic resonance) and Josephson-junction-based systems.

Let T be a sufficiently large evolution time, as predicated by the gap and the magnitude of the matrix elements $\langle n|\frac{\partial H}{\partial t}|k\rangle$, and let the normalized time be s=t/T. Then the total Hamiltonian takes the form $H(s)=a(s)H_0+b(s)H_p$, where the functions a and b are monotonically decreasing and increasing, respectively, and $a(0)=1, \ a(1)=0, \ \text{and} \ b(0)=0 \ \text{and} \ b(1)=1.$ A key requirement is that the initial H_0 and problem H_p Hamiltonians do not commute, lest the gap may vanish. There is an infinite number of choices of the functions a and b, and, furthermore, a full Hamiltonian such as $H(s)=a(s)H_0+c(s)H_a+b(s)H_p$ with c(0)=c(1)=0 with additional term H_a is certainly possible. For the purpose of concreteness in

implementation we will later restrict to $H(s) = (1 - s)H_0 + sH_p$. However, it may be noted that using such a linear interpolation does not provide a computational advantage for quantum search, and that a rescaling is required in order to obtain the optimality of Grover's algorithm [13].

A convenient, restricted, and certainly not universal class of Hamiltonians is the Ising model

$$H = -\sum_{i} h_i \sigma_z^i - \sum_{i < j} J_{ij} \sigma_z^i \sigma_z^j, \tag{1}$$

where h_i correspond to magnetic field strengths and J_{ij} to spin-spin couplings. In particular, there are no transverse field contributions to this class of problem Hamiltonians, and it is 2-local: there are no interactions of 3 or more spins. The model (1) conveniently extends semiclassical magnetic models with spins $s_i = \pm 1$ to the quantum domain with operators $\sigma_z^i = \text{diag}(1, -1)$ acting on the *i*th qubit.

Again there is much choice in the initial Hamiltonian H_0 . One such that is very convenient, but not necessarily providing the best behavior of the spectral gap, is $H_0 = -h_0 \sum_i \sigma_x^i$, where σ_x^i is the NOT gate on the *i*th qubit. Among many others, $H_0 = -h_0 \sum_{i < j} \sigma_x^i \sigma_x^j$ is an alternative.

In the following sections, we set up and illustrate the knapsack problem, commenting on classical algorithms, then describe high-level implementations for Ising models for an AQC solution. We also discuss the AQC solution of some other, more restricted problems.

Concerning NP-difficult combinatorial optimization problems, these require an exponentially large amount of at least one resource for solution in the worst case, and the AQC methodology will not always provide an advantage [17]. With N a measure of problem size, the computational cost may then vary as $O[\exp(\alpha N^{\beta})]$ for very large N and positive α and β . When the AQC approach is more effective than classical algorithms, we expect as a result the exponent αN^{β} to typically be reduced to $\alpha N^{\beta}/2$. While a further reduction in computational cost would be appealing, this

is still very significant for practical-size problems.

The Knapsack problem

We will be concerned with knapsack instances with integer weights w_j and profits p_j . The input for the knapsack problem consists of these numbers together with a capacity c, also taken to be an integer, and n, the number of items. Formulated as a binary programming problem, knapsack then is comprised as follows.

$$(KP)$$
 maximize $\sum_{j=1}^{n} p_j x_j$
subject to $\sum_{j=1}^{n} w_j x_j \le c$,

with $x_j \in \{0,1\}$ for $1 \leq j \leq n$. The knapsack problem and its various extensions have numerous applications in packing and stock cutting problems, financial decision making, asset-backed securitization, and combinatorial auctions [8]. In the latter area, a bundle of goods is sold, not just a single item. Moreover, solutions of knapsack may serve to find a solution of a more complicated problem, which could include scheduling.

The special case of $p_j = w_j$ for j = 1, ..., n is referred to as the subset sum problem. It is still NP difficult. Although many algorithms for knapsack are suitable for it, it may also be attacked by more specialized means.

Some remarks on the input for the knapsack problem are in order, beyond that we take $n \geq 2$. For each weight we require $w_j \leq c$, and for their sum $\sum_{j=1}^n w_j > c$. If the latter condition did not hold, we would simply take $x_j = 1$ for j = 1, ..., n. In addition, without loss of generality we may assume $p_j > 0$ and $w_j > 0$ for j = 1, ..., n. If otherwise a value p_k or w_k is negative, the problem instance may be manipulated in order to have positive weights and profits.

For the knapsack problem, as with other NP difficult problems, we expect that there is one or more phase transitions in problem difficulty. We may expect that in some sense average problem instances are easy and only require polynomial amounts of computational resources, but that certain subsets, as with weights and/or costs with a large least common multiple require exponential amounts of resource. For the easier number partitioning problem, the question of a phase transition has been fairly well studied and characterized [4, 5, 12, 14, 15]. If for the knapsack problem the weights are drawn from $\{1, 2, ..., L_w\}$ and the profits from $\{1, 2, ..., L_p\}$, then two of the parameters describing the phase transition(s) may be $\kappa_w = \log_2 L_w/n$ and $\kappa_p = \log_2 L_p/n$, yet the capacity must also be brought in. Section 4.3 of the review [16] may be consulted for a discussion of instance difficulty for knapsack. In the Appendix we include analytic results which complement the analysis of hard versus easy cases of a subset sum problem.

As an illustration of knapsack, and which will also serve as a test case in the next section, we consider an instance with n = 7 and c = 9:

j					5	6	7
p_j	6	5	8	9	6	7	3
$y_j \\ w_j$	2	3	6	7	5	8	4

The items have been listed in decreasing order of efficiency ratio $r_j = p_j/w_j$. Accordingly, greedy algorithms will return a solution of either items 1 and 2 with profit 11 or items 1, 2, and 7 with profit 14. However, the optimal solution with profit value 15 comes from items 1 and 4.

In addition to greedy algorithms and branch-and-bound, a classical algorithm that may be used to solve knapsack is dynamic programming (DP) by weights or by profits. When using DP by weights, a series of problems for capacity values d = 0, ..., c computes profit values $z_j(d)$. Then a certain recursion is applied for j = 1 up to j = n, yielding the optimum solution value as $z_n(c)$. I.e., the all-capacities knapsack problem is solved in this procedure. With returning the optimal profit value z^* but not explicitly the optimal solution set of items, the running time is O(nc).

AQC solution via Ising models

We present two versions of a problem Hamiltonian for the knapsack problem as formulated in [11]. The second form is implicit in [11] so that we provide more explanation for it. We have implemented both of these Hamiltonians in Mathematica[©]

together with initial Hamiltonians in order to produce a simulation of the spectral gap.

Firstly let x_i be binary variables for $1 \le i \le n$ and y_k be binary variables for $1 \le k \le c$. A problem Hamiltonian may be written as $H = H_A + H_B$, where

$$H_A = A \left(1 - \sum_{j=1}^c y_j \right)^2 + A \left(\sum_{j=1}^c j y_j - \sum_{i=1}^n w_i x_i \right)^2, \tag{2a}$$

and

$$H_B = -B\sum_{i=1}^n p_i x_i. (2b)$$

The term H_B serves to maximize the profit and the term H_A ensures that the total weight constraint is satisfied. In this set up, only a single y_j variable will be nonzero. The condition on A and B is $0 < B\max(p_j) < A$. The number of qubits required is n + c, the sum of the number of items and the capacity. In the quantum version the binary variables x_i are represented by the operators $(I + \sigma_z^i)/2 = \text{diag}(1,0)$.

We now make it explicit how the number of needed qubits may be substantially reduced to $n + [\log_2 c] + 1$. Let the integer M be determined from $M = [\log_2 c]$, thus ensuring that $2^M \le c < 2^{M+1}$. The reduced problem Hamiltonian then consists still of H_B , with now

$$H_A = A \left(\sum_{j=0}^{M-1} 2^j y_j + (c+1-2^M) y_M - \sum_{i=1}^n w_i x_i \right)^2.$$
 (3)

There are now M+1 new binary variables y_0, y_1, \ldots, y_M , and generally several of them will be nonzero together. This occurs due to nonuniqueness to represent a total weight.

As an example suppose that the capacity c=10. We may quickly verify that all total weights up to c may be represented with 4 binary variables. Here M=3 and the combination $y_0+2y_1+4y_2+3y_3$ may represent all values $1, 2, \ldots, 10$. For instance, total weight 6 results for either $y_1=1=y_2$ and $y_0=0=y_3$ or $y_0=1=y_1=y_3$ and $y_2=0$. Hence degenerate ground state solutions are now possible.

We have principally used $H_0 = -h_0 \sum_i \sigma_x^i$ as the initial Hamiltonian in the simulations, where in the first version i runs from 1 to n+c, and in the second from 1 to n+M+1. Since the problem Hamiltonians are diagonal by definition, implementations with programming languages which are efficient with lists can benefit from this aspect. Comparing the Ising form (1) with (2) and (3) we see that the profits p_j and weights w_j enter the magnetic field parameters h_i and that the product of weights $w_i w_j$ contributes to the qubit-qubit couplings J_{ij} .

Figures 1a and 1b show respectively the ground state energy, first excited state energy, and their difference, and the latter difference separately for the knapsack instance with n = 5 and c = 7:

j	1	2	3	4	5
p_j	8	3	5	6	9
w_j	1	2	1	3	2

The optimal solution consists of items 1, 3, 4, and 5, with profit 28 and total weight 7 matching the capacity. The adiabatic solution is based upon using problem Hamiltonian (2) so that 12 qubits are needed. A fairly common feature with this approach is a small gap at smaller values of s, followed by a very nearly linear behavior.

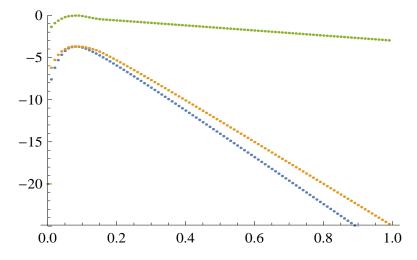


Figure 1: Fig. 1a. Ground and first excited state energies, and their difference, vs s=t/T.

An example for the gap of the test problem of the previous section is given in Figs. 2a and 2b. Here the problem Hamiltonian is based upon (2b) and (3). Again

Energy Gap for Adiabatic Hamiltonian E 0.0 -0.5 -1.0 -1.5 -2.0 0.0 0.2 0.4 0.6 0.8 1.0 s=t/T

Figure 2: Fig. 1b. Energy difference of the first and ground states energies vs s=t/T.

the energy difference between the ground and first excited states is smallest for the earlier times. This seems to be a fairly generic feature, but some problem instances have the smallest such difference at significantly larger values of s.

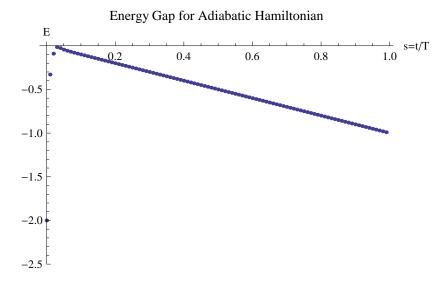


Figure 3: Fig. 2a. Energy difference of the first and ground states energies vs s=t/T.

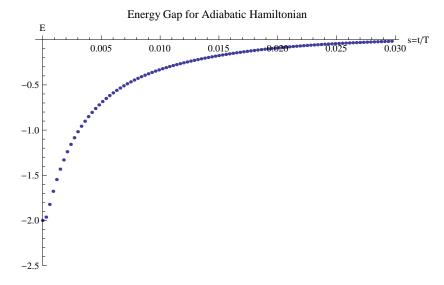


Figure 4: Fig. 2b. Energy difference of the first and ground states energies vs s=t/T.

Discussion of a version of quantum search

The concluding section of [11] gives a problem Hamiltonian in terms of binary variables x_i for determining the largest integer in a set n_1, n_2, \ldots, n_N ,

$$H = A \left(1 - \sum_{i} x_i\right)^2 - B \sum_{i} n_i x_i. \tag{4}$$

The term with coefficient B causes the largest integers to enter the sum, while this is counterbalanced by the term with coefficient A to include the sole largest. The condition for this Ising model to solve the problem is $A > B \max_i(n_i)$. However, the quantity on the right side of this inequality is not known a priori, and is in fact the sought-for solution. This means that in practice A might have to be taken arbitrarily large, and this would very likely lead to a small gap for all initial Hamiltonians. In turn, this implies that it is not as easy as at first glance to recover the optimal order $O(\sqrt{N})$ of quantum search. We recall as in the Introduction that a modified evolution schedule for AQC is required to recover the optimal running time [13]. Thus, it is correct that AQC may also solve computationally easy problems, but this approach does not guarantee an advantage over classical algorithms.

Figure 3a shows the gap for an evolution starting with the initial Hamiltonian $H_0 = -\sum_i \sigma_x^i$ and ending with that of (4) for only three positive integers, with the

largest being 6. For the vast majority of the time the gap is very close to linear in s. However, for small values of s, as shown in Fig. 3b, there is an abrupt decrease to the global minimum before the start of the linear growth. For six positive integers, the largest being 91, the behavior of the gap is very similar, as shown in Figs. 4a and 4b.

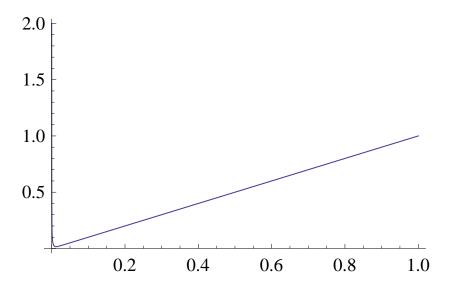


Figure 5: Fig. 3a. Energy difference of the first and ground states energies vs s=t/T for 3 input integers to be searched.

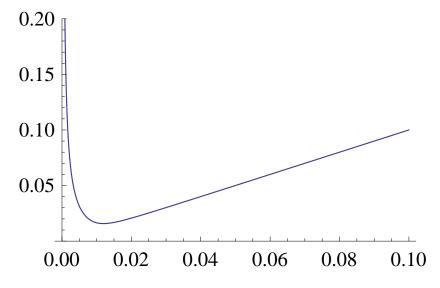


Figure 6: Fig. 3b. Energy difference of the first and ground states energies vs $s=t/T\leq 0.1.$

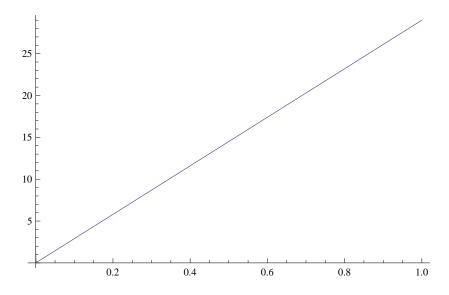


Figure 7: Fig. 4a. Energy difference of the first and ground states energies vs s=t/T for 6 input integers to be searched.

Summary

In summary, we have illustrated the AQC solution of the knapsack problem with both integer profits and weights. Indeed, it is the integrality condition of these quantities when maximizing the profit subject to an integer capacity c that leads to the NP complexity of the problem. We have given specific examples using both a problem Hamiltonian requiring n + c qubits for n items and a much more efficient one using $n + [\log_2 c] + 1$ qubits. Our limited numerical evidence shows that often the spectral difference between the ground and first excited states has a minimum at small values of the normalized time s = t/T. It would be of interest to know how the gap behaves with problem size. In particular, if it could be shown that the gap decreases only polynomially (i.e., not exponentially) for larger and larger problems, then the efficiency of the AQC approach would be verified. On the numerical side, this would very likely require an implementation in a compiled computer language and the running of a large number of cases, given that all of the profits, weights, and capacity are subject to variation. ¹ Thus further theoretical analysis is also of interest, which might be approached by first restricting to certain classes of knapsack problems.

¹And this is even in regard to a fixed initial Hamiltonian.

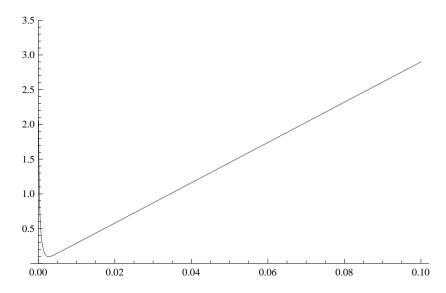


Figure 8: Fig. 4b. Energy difference of the first and ground states energies vs $s=t/T\leq 0.1.$

Statistical mechanical analyses of the knapsack problem have been very limited. In particular, both of the works [9] and [7] have taken all of the profits p_j to have the same constant value. The latter article treats multiple constraints for continuous knapsack variables but the number of constraints is directly proportional to the number of items and the investigation focuses on the capacity being one fourth of the number of items.

We have verified the Ising model problem Hamiltonians, as expected. Of further interest would be alternative Hamiltonians requiring less 'connectivity', i.e., fewer spin-spin couplings. Interestingly enough, though, there has been a recent experimental proposal for adiabatic quantum optimization based upon ion traps, and it is thought that a variety of knapsack problems could be solved within this framework [6]. This scheme is described as possible with current trapped-ion technology by adjusting local laser intensities, in contrast to requiring specially designed trapping potentials or a large number of laser frequencies. In addition, it has been shown that at the expense of using $O((n + [\log_2 c])^2)$ qubits, as a special case of an all-to-all coupled Ising model, only local interactions in a square-lattice arrangement are required [10]. Thus, nearer-term experimental implementation may be within reach.

The subset sum problem, a very special case of knapsack, extends the number partitioning problem. Within the Appendix we develop additional analytic expressions which serve to characterize the transition from easy to hard instances of the subset sum problem.

Acknowledgements

The assistance of O. Orejola is gratefully acknowledged. In turn, his support from the Colorado School of Mines Multicultural Engineering Program during the summer of 2016 is also. Dr. P. Hauke is thanked for reading the manuscript.

Appendix: Relations for a subset sum problem

In [14] the authors consider the integer solutions of H = E, where $H = \sum_{j=1}^{N} a_j n_j$. Here the a_j 's are given positive integers and the n_j 's, each taking the values 0 and 1, form the solution(s), if they exist. We supplement the asymptotic analysis of section 4 of [14] which uses W(E), the number of solutions of the problem H = E.

Let the a_j 's be drawn uniformly from the set $\{1, 2, ..., L\}$ and let $\alpha = \beta/L$ be a scaled inverse temperature. In the limit of $N \to \infty$ with L fixed, by replacing a summation with an integral there results

$$x = \frac{E}{NL} \approx \int_0^1 \frac{ydy}{1 + e^{\alpha y}}.$$

The parameter describing whether at least one solution of the subset sum problem exists is $\kappa = \log_2 L/N$. In the limit of N and $L \to \infty$, the condition W(E) = 1 gives the critical value

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

This quantity separates the regions of hard versus easy instances of the randomized subset sum problem, with $\kappa > \kappa_c$ being the hard-to-solve region.

We first prove certain symmetries which are implicit in Figure 2 of section 4 of [14]. Then we make use of the dilogarithm function $\text{Li}_2(z)$ to write the functions $x = x(\alpha)$ and $\kappa_c = \kappa_c(\alpha)$. The latter expressions, as we indicate, provide an alternative means to show the first Proposition.

Proposition 1. Let $-\infty < \alpha < \infty$. Then (a) $x(\alpha) + x(-\alpha) = 1/2$, and (b) $\kappa_c(\alpha) = \kappa_c(-\alpha)$.

Hence the phase transition for this subset sum problem is determined once x and κ_c are known for say the interval $0 \le \alpha < \infty$.

Proof. (a) We immediately have

$$x(\alpha) + x(-\alpha) = \int_0^1 y dy = \frac{1}{2}.$$

(b) We may write

$$\kappa_c(\alpha) = \frac{1}{\ln 2} \left[\int_0^1 \ln(1 + e^{-\alpha y}) dy + \alpha x(\alpha) \right].$$

We have

$$\int_0^1 \ln\left(\frac{1+e^{-\alpha y}}{1+e^{\alpha y}}\right) dy = -\alpha \int_0^1 y dy = -\frac{\alpha}{2}.$$

Then by part (a), part (b) follows since the relation $\kappa_c(\alpha) - \kappa_c(-\alpha) = 0$ is equivalent to

$$\frac{1}{\ln 2} \left[\alpha(x(\alpha) + x(-\alpha)) - \frac{\alpha}{2} \right] = 0.$$

It is also of interest to separately write the functions $x(\alpha)$ and $\kappa_c(\alpha)$. For this, we introduce the analytically continuable dilogarithm function $\text{Li}_2(z) = \sum_{n=1}^{\infty} z^n/n^2$ ($|z| \leq 1$). In particular, $\text{Li}_2(-1) = -\pi^2/12$ and among others, there are the functional relations

$$\operatorname{Li}_{2}\left(-\frac{1}{x}\right) + \operatorname{Li}_{2}(-x) = 2\operatorname{Li}_{2}(-1) - \frac{1}{2}\ln^{2}x,$$
 (A.1)

and

$$\text{Li}_2(z) + \text{Li}_2(1-z) = \frac{\pi^2}{6} - \ln z \ln(1-z).$$
 (A.2)

Proposition 2. Let $-\infty < \alpha < \infty$. Then (a)

$$x(\alpha) = -\frac{\pi^2}{12\alpha^2} + \frac{1}{2} - \frac{1}{\alpha}\ln(1 + e^{\alpha}) - \frac{1}{\alpha^2}\text{Li}_2(-e^{\alpha}),$$

and (b)

$$\kappa_c(\alpha) = -\frac{1}{\ln 2} \left[\frac{\alpha}{2} + \frac{\pi^2}{12\alpha} + \frac{1}{\alpha} \text{Li}_2(-e^{\alpha}) - \alpha x \right].$$
$$= -\frac{1}{\ln 2} \left[\frac{\pi^2}{6\alpha} + \frac{2}{\alpha} \text{Li}_2(-e^{\alpha}) + \ln(1 + e^{\alpha}) \right].$$

Proof. For both parts we proceed by using power series expansion of the integrands for the subject functions. For (a),

$$x = \frac{E}{NL} \approx \int_0^1 \frac{ydy}{1 + e^{\alpha y}} = \sum_{m=0}^{\infty} (-1)^m \int_0^1 e^{-\alpha(m+1)y} ydy$$

$$= \sum_{m=0}^{\infty} \frac{(-1)^m}{\alpha^2} \left[\frac{1}{(m+1)^2} - \frac{e^{-\alpha(m+1)}}{(m+1)^2} (\alpha(m+1)+1) \right]$$

$$= -\frac{1}{\alpha^2} \text{Li}_2(-1) - \frac{1}{\alpha^2} \sum_{m=0}^{\infty} (-1)^m \frac{e^{-\alpha(m+1)}}{(m+1)^2} - \frac{1}{\alpha} \sum_{m=0}^{\infty} \frac{(-1)^m e^{-\alpha(m+1)}}{m+1}$$

$$= \frac{\pi^2}{12\alpha^2} - \frac{1}{\alpha^2} \text{Li}_2(-e^{-\alpha}) - \frac{1}{\alpha} \ln(1+e^{-\alpha}).$$

For (b) we use the integral

$$\int_{0}^{1} \ln(1 + e^{-\alpha y}) dy = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \int_{0}^{1} e^{-\alpha k y} dy$$
$$= \sum_{k=1}^{\infty} \frac{(-1)^{k}}{k^{2}} (1 - e^{-\alpha y})$$
$$= \frac{\pi^{2}}{12\alpha} + \frac{1}{\alpha} \text{Li}_{2}(-e^{-\alpha})$$
$$= -\frac{\alpha}{2} - \frac{\pi^{2}}{12\alpha} - \frac{1}{\alpha} \text{Li}_{2}(-e^{\alpha}).$$

The latter expression follows from (A.1).

An alternative proof of Proposition 2 may be based upon the integral representation

$$\operatorname{Li}_{2}(z) = -\int_{0}^{z} \frac{\ln(1-t)}{t} dt,$$

as, with a change of variable, we have

$$x(\alpha) = \frac{1}{\alpha^2} \int_2^{1+e^{\alpha}} \frac{\ln(u-1)du}{u(u-1)} = \frac{1}{\alpha^2} \int_2^{1+e^{\alpha}} \left(-\frac{1}{u} + \frac{1}{u-1}\right) \ln(u-1)du.$$

Upon evaluation of the integrals and the use of (A.2), the results of Proposition 2 may again be obtained.

It is now apparent how the explicit expressions of Proposition 2 may be used to verify the symmetries of Proposition 1. For example, for part (b) there we have, using relation (A.1),

$$\kappa_c(-\alpha) = \frac{1}{\ln 2} \left[\frac{\pi^2}{6\alpha} + \frac{2}{\alpha} \text{Li}_2(-e^{-\alpha}) - \ln(1 + e^{-\alpha}) \right]$$
$$= \frac{1}{\ln 2} \left[\frac{\pi^2}{6\alpha} + \frac{2}{\alpha} \left[-\text{Li}_2(-e^{\alpha}) - \frac{\pi^2}{6} - \frac{\alpha^2}{2} \right] - \ln(1 + e^{-\alpha}) \right]$$

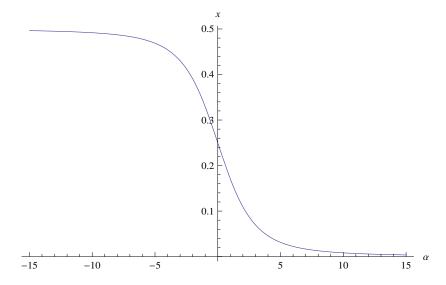


Figure 9: Fig. 5a. The function x = E/(NL) is plotted versus $\alpha = \beta/L$.

$$= \frac{1}{\ln 2} \left[-\frac{\pi^2}{6\alpha} - \frac{2}{\alpha} \operatorname{Li}_2(-e^{\alpha}) - \alpha - \ln(1 + e^{-\alpha}) \right] = \kappa_c(\alpha).$$

Figure 5(a) shows a plot of x versus α and (b) a plot of κ_c versus α .

The identification of x and κ_c in terms of the dilogarithm function is also useful in that other points may be obtained exactly. In particular, for $\alpha_{\mp} = \frac{1}{2} \ln(\mp 1 + \sqrt{5})$,

$$\operatorname{Li}_{2}(-e^{\alpha_{-}}) = -\frac{\pi^{2}}{15} + \frac{1}{2}\ln^{2}\left(\frac{\sqrt{5}-1}{2}\right),$$

and

$$\operatorname{Li}_{2}(-e^{\alpha_{+}}) = -\frac{\pi^{2}}{10} + \frac{1}{2}\ln^{2}\left(\frac{\sqrt{5}+1}{2}\right).$$

These then give closed form evaluations of $x(\alpha_{\mp})$ and $\kappa_c(\alpha_{\mp})$.

We may now describe the curve x versus κ_c in special important regions.

Proposition 3. (a) About x = 1/4 and $\kappa_c = 1$ there holds

$$x(\kappa_c) = \frac{1}{12} (3 \pm 2\sqrt{6 \ln 2} \sqrt{1 - \kappa_c}).$$

(b) For x and κ_c near zero, there holds

$$x(\kappa_c) = \frac{12}{49} (\ln^2 2) \kappa_c^2.$$

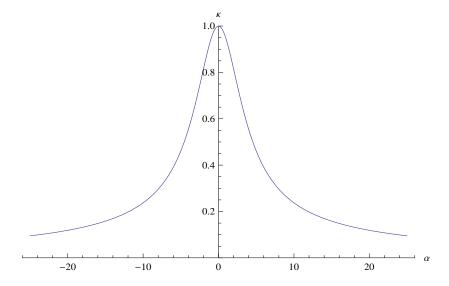


Figure 10: Fig. 5b. The function κ_c is plotted versus $\alpha = \beta/L$.

Proof. (a) This region is characterized by $\alpha \to 0$ and accordingly we have the expansion

$$x(\alpha) = \frac{1}{4} - \frac{\alpha}{12} + O(\alpha^3).$$

Then $\alpha \simeq 3(1-4x)$, while

$$\kappa_c(\alpha) = 1 - \frac{\alpha^2}{24 \ln 2} + O(\alpha^3).$$

By inverting the relation

$$\kappa_c(x) \simeq 1 - \frac{3}{8} \frac{(1 - 4x)^2}{\ln 2}$$

we obtain the stated expression.

(b) corresponds to $\alpha \to \infty$, in which case $x(\alpha) \sim 3/(4\alpha^2)$. This is inserted into the approximation

$$\kappa_c \approx \frac{1}{\log 2} \left[\alpha x(\alpha) + \frac{1}{\alpha} (1 - e^{-\alpha}) \right],$$

where the last term may be ignored in comparison to the others. This gives

$$\kappa_c \approx \frac{1}{\log 2} \left(\frac{\sqrt{3}}{2} + \frac{2}{\sqrt{3}} \right) \sqrt{x},$$

and rearranging provides the result.

There are differential relations between the scaled energy and the critical value κ_c . For example, we have the following.

Proposition 4. There holds

$$\kappa_c(\alpha) = \frac{1}{\ln 2} \int \alpha dx(\alpha).$$

Proof. We have

$$x(\alpha) = -\frac{d}{d\alpha} \int_0^1 \ln(1 + e^{-\alpha y}) dy,$$

yielding

$$x(\alpha) = -\frac{d}{d\alpha}[(\ln 2)\kappa_c(\alpha) - \alpha x(\alpha)].$$

Then

$$\alpha \frac{dx(\alpha)}{d\alpha} = (\ln 2) \frac{d\kappa_c(\alpha)}{d\alpha},$$

giving the result.

Therefore, from $dx/d\kappa_c = (\ln 2)/\alpha$ we know that the $x - \kappa_c$ curve has negative slope for $\alpha < 0$ and positive slope for $\alpha > 0$.

We may also mention the constrained subset sum problem, for which the number of chosen a_j 's is fixed to an integer M > 0, so that now $\sum_{j=1}^{N} n_j = M$. In this setting, the statistical mechanical analysis uses the grand canonical ensemble [15] with chemical potential $\mu > 0$.

We introduce the following quantities 2

$$\rho = \frac{M}{N} \approx \int_0^1 \frac{dy}{1 + e^{\alpha y - \mu}}, \quad x = \frac{E}{NL} \approx \int_0^1 \frac{y dy}{1 + e^{\alpha y - \mu}},$$

and the critical value

$$\kappa_c(\alpha) = \frac{1}{\ln 2} \int_0^1 \left[\ln(1 + e^{-\alpha y + \mu}) + \frac{\alpha y}{1 + e^{\alpha y - \mu}} - \frac{\mu}{1 + e^{\alpha y - \mu}} \right] dy.$$

We now have the following mathematical symmetries:

$$\rho(-\alpha, \mu) + \rho(\alpha, \mu) = 1,$$

²With $\alpha = \beta/L$ as before, despite the first line of p. 371 of [15].

$$x(\alpha, \mu) + x(-\alpha, -\mu) = \frac{1}{2},$$

and

$$\kappa_c(\alpha, \mu) = \kappa_c(-\alpha, -\mu).$$

We omit proofs of these relations as well as of explicit expressions which we supply next.

For
$$\rho = M/N$$
, ³

$$\rho = 1 - \frac{1}{\alpha} \ln \left(\frac{1 + e^{-\mu}}{1 + e^{\alpha - \mu}} \right).$$

For the scaled energy,

$$x(\alpha, \mu) = \frac{1}{2\alpha} \left[\alpha - 2 \ln(1 + e^{\alpha - \mu}) \right] + \frac{1}{\alpha^2} \left[\text{Li}_2(-e^{-\mu}) - \text{Li}_2(-e^{\alpha - \mu}) \right].$$

For the critical value κ_c , for which $\kappa > \kappa_c$ is a region of hard problem instances for the constrained subset sum problem,

$$\kappa_c(\alpha,\mu) = \frac{1}{\ln 2} \left\{ -\ln(1+e^{\alpha-\mu}) + \frac{2}{\alpha} \left[\operatorname{Li}_2(-e^{-\mu}) - \operatorname{Li}_2(-e^{\alpha-\mu}) \right] \right\}.$$

We also omit expressions for the number of solutions W(E, M) of the constrained problem. These may be written in terms of the logarithm, dilogarithm, and trilogarithm functions. The reduction of the expressions for $x(\alpha, \mu)$ and $\kappa_c(\alpha, \mu)$ as $\mu \to 0$ for the unconstrained case is obvious.

³Note accordingly that a correction for an exponent in the expression for $\mu = \mu(\alpha, \rho)$ on p. 371 of [15] is needed.

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