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Quantum Statistical Mechanics on a Quantum Computer

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We describe a quantum algorithm to compute the density of states and thermal equilibrium properties of quantum many-body systems. We present results obtained by running this algorithm on a software implementation of a 21-qubit quantum computer for the case of an antiferromagnetic Heisenberg model on triangular lattices of different size.

§1. Introduction

Recent theoretical work has shown that a Quantum Computer (QC) has the potential of solving certain computationally hard problems such as factoring integers and searching databases much faster than a conventional computer. ¹⁾⁻⁶ The idea that a QC might be more powerful than an ordinary computer is based on the notion that a quantum system can be in any superposition of states and that interference of these states allows exponentially many computations to be done in parallel.⁷ This hypothetical power of a QC might be used to solve other difficult problems as well, such as for example the calculation of the physical properties of quantum manybody systems.⁸⁾⁻¹⁰⁾ As a matter of fact, part of Feynman's original motivation to consider QC's was that they might be used as a vehicle to perform exact simulations of quantum mechanical phenomena.¹¹⁾ For future applications it is clearly of interest to address the question how to program a QC such that it performs a simulation of specific physical systems.

In this paper we describe a quantum algorithm (QA) to compute the equilibrium properties of quantum systems by making a few statistically uncorrelated runs, starting from random initial states. Exploiting the intrinsic parallellism of the hypothetical QC this QA executes in polynomial time. En route this QA computes the density of states (DOS) from which all the eigenvalues of the model Hamiltonian may be determined. We test our QA on a software implemention of a 21-qubit QC by explicit calculations for an antiferromagnetic Heisenberg model on a triangular

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lattice.

§2. Theory

Consider the problem of computing the physical properties of a quantum system, described by a Hamiltonian H, in thermal equilibrium at a temperature T. In the canonical ensemble this equilibrium state is characterised by the partition function $Z = \text{Tr} \exp(-\beta H)$ where $\beta = 1/k_B T$ and k_B is Boltzmann's constant (we put $k_B = 1$ and $\hbar = 1$ in the rest of this paper). The dimension of the Hilbert space of physical states will be denoted by D. If all the eigenvalues $\{E_i; i = 1, \ldots, D\}$ of H are known, we can make use of the fact that $Z = \sum_{i=1}^{D} \exp(-\beta E_i)$ to reduce the computation of the physical properties to a classical statistical mechanical problem which can be solved by standard probabilistic methods.¹²⁾ For a non-trivial quantum many-body system the determination of the eigenvalues is a difficult computational problem itself, in practice as difficult as the calculation of Z. In view of this we will from now on assume that the eigenvalues of H are not known.

The DOS

$$\mathcal{D}(\epsilon) = \sum_{i} \delta(\epsilon - E_i) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{it\epsilon} \operatorname{Tr} e^{-itH} dt, \qquad (1)$$

determines the equilibrium state of the system. Indeed, once $\mathcal{D}(\epsilon)$ is known Z is easy to calculate:

$$Z = \int_{-\infty}^{+\infty} e^{-\beta\epsilon} \mathcal{D}(\epsilon) \, d\epsilon.$$
 (2)

Integral (2) exists whenever the spectrum of H has a lowerbound, i.e. $\mathcal{D}(\epsilon) = 0$ for $-\infty < \epsilon < \min_i E_i$. Note that $\mathcal{D}(\epsilon)$ is a real-valued function.

With suitable (time-dependent) modifications of H, the partition function plays the role of a generating function from which all physical quantities of interest can be obtained. Physical quantities such as the energy and specific heat are given by

$$E = \langle H \rangle = \frac{1}{Z} \int_{-\infty}^{+\infty} \epsilon e^{-\beta \epsilon} \mathcal{D}(\epsilon) \, d\epsilon, \qquad (3)$$

and

$$C = \beta^2 (\langle H^2 \rangle - \langle H \rangle^2) = \beta^2 \left(\frac{1}{Z} \int_{-\infty}^{+\infty} \epsilon^2 e^{-\beta \epsilon} \mathcal{D}(\epsilon) \, d\epsilon - E^2 \right), \tag{4}$$

respectively.

From (1) it is clear that the computation of $\mathcal{D}(\epsilon)$ consists of two parts: 1) Compute the trace of e^{-itH} for many values of t and 2) perform a (Fast) Fourier Transform of this data. It is known how to carry out part 2 on a QC^{7), 13)-15)} so we focus on part 1.

The QA described below computes $e^{-itH}|\psi\rangle$ for any ψ in $\mathcal{O}(\log D)$ operations. We now argue that in practice it will usually be sufficient to determine a small fraction ($\approx \mathcal{O}(\log D)$) of the D diagonal matrix elements of e^{-itH} . Instead of computing diagonal matrix elements with respect to a chosen complete set of basis states $\{\phi_n; n = 1, ..., D\}$, we generate random numbers $\{a_n; n = 1, ..., D\}$ and construct the new state

$$|\Phi\rangle = \sum_{n=1}^{D} a_n |\phi_n\rangle.$$
(5)

The corresponding diagonal element of the time-evolution operator reads

$$\langle \Phi | e^{-itH} \Phi \rangle = \sum_{n,m=1}^{D} a_n^* a_m \langle \phi_n | e^{-itH} \phi_m \rangle.$$
 (6)

If we now generate the a_i 's such that $\overline{a_n^* a_m} = \delta_{n,m}$ (\overline{x} denotes the average of x over statistically independent realizations) then

$$\overline{\langle \Phi | e^{-itH} \Phi \rangle} = \sum_{n=1}^{D} \langle \phi_n | e^{-itH} \phi_n \rangle = \text{Tr}e^{-itH}.$$
(7)

In other words, the trace of the time-evolution operator can be estimated by random sampling of the states $|\Phi\rangle$.¹⁶

A QC computes $|e^{-itH}\Phi\rangle$ just as easily as $|e^{-itH}\phi_m\rangle$ and in practice there would be no need to have a random state generator: Switching the QC off and on will put the QC in some random initial state. However to compute $\langle \Phi | e^{-itH}\Phi \rangle$ we would have to store the initial state $(|\Phi\rangle)$ in the QC and project $|e^{-itH}\Phi\rangle$ onto it, a rather complicated procedure. Instead it is more effective to apply to $|\phi_1\rangle$ a random sequence of Controlled-NOT operations to construct e.g. an entangled random state $|\Phi\rangle = D^{-1/2}(\pm\phi_1 \pm \phi_2 \dots \pm \phi_D)$.^{14), 17)} We then calculate $|e^{-itH/2}\Phi\rangle = \sum_{n=1} b_n(t/2)|\phi_n\rangle$ and use

$$\langle \Phi | e^{-itH} \Phi \rangle = \langle e^{itH/2} \Phi | e^{-itH/2} \Phi \rangle = \sum_{n=1}^{D} b_n^2(t/2) \tag{8}$$

to obtain the diagonal matrix element. Each of these steps executes very efficiently on a QC.

Remains the question how many samples S are needed to compute the energy and specific heat to high accuracy. According to the central limit theorem the statistical error on the results vanishes as $1/\sqrt{S}$. However, as we demonstrate below, the application of our QA to a highly non-trivial quantum many-body system provides strong evidence that this error also **decreases** with the system size. For systems of 15 qubits or more, we find that taking S = 20 samples already gives very accurate results. Our experimental finding that the statistical error on $\langle \Phi | e^{-itH} \Phi \rangle$ for randomly chosen $|\Phi\rangle$ decreases with D gives an extra boost to the efficiency of the QA.

§3. Soft Quantum Computer and Quantum Algorithm

The method described above has been tested on our Soft Quantum Computer (SQC). The SQC used to compute the results presented in the present paper is a

H. De Raedt et al.

hard-coded version, derived from of a more versatile SQC discussed elsewhere.¹⁸⁾ Our SQC solves the time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle,\tag{9}$$

for a quantum many-body system described by the spin-1/2 Hamiltonian

$$H = -\sum_{i,j=1}^{L} \sum_{\alpha=x,y,z} J_{i,j}^{\alpha} S_{i}^{\alpha} S_{j}^{\alpha} - \sum_{i=1}^{L} \sum_{\alpha=x,y,z} h_{i}^{\alpha} S_{i}^{\alpha},$$
(10)

where the first sum runs over all pairs P of spins (qubits), S_i^{α} ($\alpha = x, y, z$) denotes the α -th component of the spin-1/2 operator representing the *i*-th spin, $J_{i,j}^{\alpha}$ determines the strength of the interaction between the spins at sites *i* and *j*, and h_i^{α} is the (local magnetic) field acting on the *i*-th spin. The number of qubits is L and $D = 2^L$. Hamiltonian (10) is sufficiently general to capture the salient features of most physical models of QC's (our SQC also deals with time-dependent external fields).

According to (9) the QC will evolve in time through the $D \times D$ unitary transformation $U(t) = e^{-itH}$. We now describe the QA that computes $U(t)|\Phi\rangle$ for arbitrary $|\Phi\rangle$. Using the semi-group property of U(t) to write $U(t) = U(\tau)^m$ where $t = m\tau$, the main step is to replace $U(\tau)$ by a symmetrized product-formula approximation.¹⁹⁾ For the case at hand it is expedient to take

$$U(\tau) \approx \widetilde{U}(\tau) = e^{-i\tau H_z/2} e^{-i\tau H_y/2} e^{-i\tau H_x} e^{-i\tau H_y/2} e^{-i\tau H_z/2},$$
 (11)

where

$$H_{\alpha} = -\sum_{i,j=1}^{L} J_{i,j}^{\alpha} S_{i}^{\alpha} S_{j}^{\alpha} - \sum_{i=1}^{L} h_{i}^{\alpha} S_{i}^{\alpha} \quad ; \quad \alpha = x, y, z.$$
(12)

Evidently $\widetilde{U}(\tau)$ is unitary and hence the algorithm to solve the TDSE is unconditionally stable.¹⁹⁾

As basis states $\{|\phi_n\rangle\}$ we take the direct product of the eigenvectors of the S_i^z (i.e. spin-up $|\uparrow_i\rangle$ and spin-down $|\downarrow_i\rangle$). In this basis, $e^{-i\tau H_z/2}$ changes the input state by altering the phase of each of the basis vectors. As H_z is a sum of pair interactions it is trivial to rewrite this operation as a direct product of 4x4 diagonal matrices (containing the interaction-controlled phase shifts) and 4x4 unit matrices. Still working in the same representation, the action of $e^{-i\tau H_y/2}$ can be written in a similar manner but the matrices that contain the interaction-controlled phase-shift have to be replaced by non-diagonal matrices. Although this does not present a real problem it is more efficient and systematic to proceed as follows. Let us denote by X(Y) the rotation by $\pi/2$ of each spin about the x(y)-axis. As

$$e^{-i\tau H_y/2} = XX^{\dagger} e^{-i\tau H_y/2} XX^{\dagger} = X e^{-i\tau H_z'/2} X^{\dagger}, \tag{13}$$

it is clear that the action of $e^{-i\tau H_y/2}$ can be computed by applying to each qubit, the inverse of X followed by an interaction-controlled phase-shift and X itself. The prime in (13) indicates that $J_{i,j}^z$ and h_i^z in H_z have to be replaced by $J_{i,j}^y$ and h_i^y respectively. A similar procedure is used to compute the action of $e^{-i\tau H_x}$.



Fig. 1. Specific heat per site as a function of the temperature.



Our SQC carries out $\mathcal{O}\left(P \, 2^L\right)$ operations to perform the transformation $e^{-i\tau H_z/2}$ but a QC operates on all qubits simultaneously and would therefore only need $\mathcal{O}\left(P\right)$ operations. The operation counts for $e^{-i\tau H_x}$ (or $e^{-i\tau H_y}$) are $\mathcal{O}\left((P+2)2^L\right)$ and $\mathcal{O}\left(P+2\right)$ for the SQC and QC respectively. On a QC the total operation count per time-step is $\mathcal{O}\left(3P+4\right)$.

§4. Application

The QA described above has been tested on our SQC by simulating the antiferromagnetic spin 1/2 Heisenberg model with J = -1 on triangular lattices of L = 6, 10, 15, 21 sites, subject to free boundary conditions. The ground-state properties of this model can be computed by standard sparse-matrix techniques, see e.g. Ref. 20). The low temperature properties of this model are difficult to compute by conventional Quantum Monte Carlo (QMC) methods.²¹⁾ The presence of frustrated interactions leads to the sign problem²¹⁾ that is very often encountered in QMC work.^{22), 23)}

In Fig. 1 we present some SQC results for the specific heat per site E/L as a function of the temperature. The number of samples S = 20 in all cases. Also shown is data obtained by exact diagonalization of H for $L = 6, 10.^{*}$) The SQC and exact results differ significantly for temperatures where the specific heat exhibits a sharp peak. This is related to the presence of a gap in the low-energy part of the spectrum and the random choice of the $|\Phi\rangle$'s. In this low-temperature regime where only a few of the lowest eigenvalues contribute, random fluctuations can have a large effect. However this is not really a problem: Knowing the DOS it is not difficult to determine the precise values of these few eigenvalues and compute Cdirectly, without invoking (4). In Fig. 2 we show results for the standard deviation (SD) on C/L, calculated from the same data. The most remarkable feature of the SD is its dependence on the system size: The larger the system, the smaller the

^{*)} The calculation of all 32768 (2097152) eigenvalues of the L = 15 (L = 21) system by standard linear algebra methods requires tremendous computational resources

SD. Unfortunately we cannot yet offer a theoretical basis for this observed decrease. At very low temperature the SD on C/L goes to zero because only one eigenstate (i.e. the ground state) effectively contributes. The large values of the L = 6, 10 low temperature SD data reflect the fact that in this regime the SQC and exact results differ considerably and indicate that for these system sizes more than S = 20 samples are necessary to obtain accurate results. On the other hand, except for test purposes, we wouldn't use a QC to simulate a 10-site system because it can easily be solved exactly on an ordinary computer.

§5. Summary

We have described a quantum algorithm to determine the distribution of eigenvalues of a quantum many-body system in polynomial time. From these data thermal equilibrium properties of the system can be computed directly. The approach has been illustrated by numerical calculations on a software emulator of a physical model of a quantum computer. Excellent results have been obtained, suggesting a new route for simulating experiments on quantum systems on a quantum computer. However, implicit in the formulation of this physical model of the quantum computer is the assumption that each physical spin represents one qubit. If this were not the case, the quantum computer will operate with much less efficiency.

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