New method for the 3D Ising model

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A simple, general and practically exact method is developed for the equilibrium properties of the macroscopic physical systems with translational symmetry. Applied to the Ising model in two and three dimension, a modest calculation gives the spontaneous magnetization and the specific heat to less than 1% error.

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To calculate the equilibrium properties of a given physical system will probably be the most basic theoretical task. In 1944, Onsager [1] calculated the partition function of the two dimensional Ising model analytically and demonstrated the power of the exact solution, followed by the exact spontaneous magnetization by Yang [2]. Since then some remarkable progresses have been made in two-dimensional classical and one-dimensional quantum systems analytically [3,4,5], and by numerical methods such as DMRG (density matrix renormalization group) [6]. However, reflecting the three-dimensionality of our world, much needed knowledge is for three dimension, and several thousand papers have been said written on the three dimensional Ising model. Among others, a tremendous effort has been paid to the precise determination of the critical temperature $T_c$ in association with the concept of universality near the critical point [7]. Owing to the concerted effort of RG-finite size scaling-Monte Carlo (MC) method, $T_c$ is known as precise as 4.5114(1) [8], as well as the spontaneous magnetization [9]. The effort of high and low temperature expansions by the diagrammatic method for $T_c$ is also remarkable [10]. Yet another noteworthy recent progress is along the line of DMRG [11].

We here present a new method for the equilibrium properties of the macroscopic physical systems with translational symmetry. Our method is purely algebraic, works directly on a $\infty \times \infty \times \infty$ lattice and, other than seeking a convergence in entanglement space (see below), it does not invoke any other notions such as numerical RG, nor make any approximations. We have calculated the spontaneous magnetization and the specific heat in two and three dimensional Ising models to less than 1% error. Note that without the help of RG, the 1% precision is what one can typically expect from exact methods such as Bethe Ansatz [3,4]. The new method is simple, general and computationally efficient. In fact, our 30 minutes calculation already gives fairly precise results as demonstrated below.

Let us consider the ferromagnetic Ising model on a square or simple cubic lattice,

$$ H = - \sum_{(i,j)} \sigma_i \sigma_j $$

where $\sigma_i$ takes + or - 1 and the summation is over the nearest neighbor pairs. The partition function is given by $Z = \text{Tr}[\exp(-\beta H)]$, where $\text{Tr}$ means to take trace over the $2^N$ spin configurations with $N$ being the number of lattice sites and $\beta = 1/kT$. We follow the following steps for the two dimensional case.

First, note that the local pair-density matrix can be written as $\exp(\beta \sigma_i \sigma_j) = \cosh(\beta) + \sinh(\beta) \sigma_i \sigma_j$. This is the simplest case of more general statement that any local density matrix when regarded as a real symmetric matrix can be written by singular value decomposition (SVD) as $A_{ij} = \sum_k V_{ik} \lambda_k V_{jk}$, where $V_k$ and $\lambda_k$ are eigenvectors and eigenvalues of the local density matrix $A$. Denoting these two terms by a "bond index" $i = 1, 2$, the partition function is written as a summation over all the bond index configurations on the square lattice. Now each term in this summation is a product over all the sites of a local spin operator constructed from $\lambda_1$ and $\lambda_2 \sigma_i$, depending on the four bond indexes surrounding the i-th spin, where $\lambda_1 = \sqrt{\cosh(\beta)}$ and $\lambda_2 = \sqrt{\sinh(\beta)}$. For example at site $i$, if the surrounding four bond indexes are all 1, then the local spin operator at the site is $\lambda_1^4$ and its trace is, $Tr \lambda_1^4 = 2\lambda_1^4$. If one of the four bond indexes is replaced by 2, then the local spin trace is, $Tr \lambda_1^4 \lambda_2 \sigma_i = 0$. Let us denote these local spin traces as $\Gamma_{ijkl}$ with the four bond indexes $i, j, k$ and $l$ taking 1 or 2. Clearly, $\Gamma_{ijkl} = 2\lambda_1^4, 2\lambda_1^2 \lambda_2^2, 2\lambda_2^4$ for $i + j + k + l = 4, 6$, and 8 respectively and zero otherwise. Performing the spin trace over all the sites, we have

$$ Z = \sum_{\text{bond}} \Pi_{\text{site}} \Gamma_{ijkl} $$

Second, by virtue of infinite system, we can conveniently assume the periodic boundary condition in both horizontal and vertical directions. Let us denote the leftmost horizontal bond indexes by a vector $a_1$ and the rightmost ones by $a_{N+1}$. The periodic boundary condition is then expressed by the Kronecker delta $\delta_{a_1 a_{N+1}}$ which can
be expanded by an orthonormal complete set \( \{ \phi_n(a) \} \) as \( \delta_{i1} \delta_{n+1} = \sum_n \phi_n(a_{1}) \phi_n(a_{N+1}) \). Note that all the quantities in this paper are real. Let us now denote the rightmost column composed of a vertical one-dimensional array of \( \Gamma \) s as \( K(a_{N}, a_{N+1}) \). Note that we can certainly regard this quantity as a function of the two bond-index vectors \( a_{N} \) and \( a_{N+1} \) after summing over the vertical bond indexes associated with this column. Now choose the above introduced eigenstate as the one which satisfies a transfer-matrix eigenvalue equation

\[
K(a_{N}, a_{N+1}) \phi_n(a_{N+1}) = \mu_n \phi_n(a_{N}) \tag{3}
\]

where and below the repeated indexes imply a summation. Repeatedly using Eq.(3), the partition function is evaluated as \( Z = \sum_n \mu_n^N \rightarrow \mu_0^N \) in the large \( N \) limit, where the suffix 0 indicates the largest eigenvalue.

The specific heat can be obtained from the free energy equation, Eq.(2).

\[
\Gamma_{ijkl} = a_{N} \Gamma_{ijkl} - \zeta_{ijkl} = \mu \Gamma_{ijkl} - \zeta_{ijkl} \]

FIG. 1: Schematic figure of the transfer matrix eigenvalue equation, Eq.(2).

that Eq.(1) is not peculiar to the Ising models, but rather a general statement for any macroscopic systems with translational symmetry. Another important note is, as is evident from the derivation above, the range of values which the entanglements \( \alpha, \beta \) and \( \gamma \) can take, grows exponentially for increasingly large systems. Thus the success of the present method crucially relies on a rapid convergence of physical quantities with the increase of entanglement. Fourth, we handle the eigenvalue problem (3) as a variational problem, namely we maximize the quantity \( \mu_0 = \varphi_0 K \varphi_0 / \varphi_0 \varphi_0 \) by iteration starting with an input state for \( \varphi_0 \). First consider the numerator. A local ingredient of this quantity is \( A_{i'} C_{mn} \). Since \( A \) is real symmetric, we can use SVD again and write as \( A = \mu e^{T} \) where the matrixes \( X \) and \( \nu \) are made up of eigenvectors and eigenvalues of \( A \) and \( t r \) means the transpose. Since \( X \) is orthogonal, the summation over the combined entanglement-bond indexes \( l'e \) in the numerator can be done for \( N-1 \) times, and thus we only keep the largest eigenvalue \( \nu_0 \) and eigenstate \( x_0 \). We have \( \varphi_0 K \varphi_0 = \nu_0^{-1} x_0 \mu e^{T} x_0 \). The denominator can be handled likewise. Let us denote the corresponding largest eigenvalue and eigenstate as \( \rho_0 \) and \( y_0 \). Note that \( \mu_0 \) now contains \( \zeta_{lmn} \) in quadratic form. Maximizing this quantity with respect to \( \zeta_{lmn} \) then leads to a generalized eigenvalue problem:

\[
x_{0} e^{T} \Gamma_{mn} f x_{0} m n = \mu_{0} x_{0} m n \implies \mu_{0} e^{T} \delta_{mn} y_{0} m n = \mu_{0} e^{T} \delta_{mn} y_{0} m n \tag{5}
\]

where \( \mu_0 = \mu_0^{-1} / \rho_0^{-1} \). We solve Eq(5) for the next \( \zeta \) and continue until convergence. Finally after the convergence, we can calculate the internal energy and spontaneous magnetization in terms of the obtained eigenvalues and eigenstates. The procedure is the same as above with only difference being one (two) of \( \Gamma \)s in the expression for the partition function should be replaced by \( \Gamma_{ijkl} = 2 \lambda_{1}^{3} \lambda_{2}, 2 \lambda_{1}^{3} \lambda_{3}^{3} \) for \( i + j + k + l = 5, 7 \) respectively and zero otherwise for calculating \( < \sigma_i > < \sigma_j > \).
We have,

$$M = x_0^{tr} \hat{A} x_0 / (\mu_0 \rho_0)$$

(6)

where $\hat{A}$ is the same as $A$ with $\Gamma$ replaced by $\hat{\Gamma}$. Likewise

$$E = -D x_0^{tr} \hat{A}^2 x_0 / (\tilde{\mu} \tilde{\rho} \nu_0)$$

(7)

The extension to three dimension is straightforward. $\Gamma$ and $\hat{\Gamma}$ now have 6 indexes, $\Gamma_{ijklmn}$ = $2 \lambda^i j k l m n$ for $i + j + k + l + m + n = 6, 8, 10$ and 12 respectively and zero otherwise and $\hat{\Gamma}_{ijklmn}$ = $2 \lambda^i j k l m n$ for $i + j + k + l + m + n = 7, 9, 11$ respectively and zero otherwise, and the bond index vector $a$ represents a two dimensional array. The largest eigenstate $\varphi_0(a)$ of the operator $K$ is now expressed as a product of $\zeta_{abcd}$, the first four indexes denoting entanglement indexes (aei), (bfj) etc. which we will denote by a single index below when possible. $B$ can then be expressed like $B_{ijkl}$.

Let us write the largest eigenvalue problem similar to Eq(3). Let us write the largest eigenvalue as $\Delta$ and the local constituent of the eigenstate as $\eta_{ttvil}$ (corresponds to $\zeta_{lmn}$ in two dimension) where the first two indexes represent the new entanglement indexes and the last a composite of bond-entanglement indexes (aei), (bfj) etc. which we will denote by a single index below when possible. $B$ can then be expressed like $B_{ijkl}$. We consider an eigenvalue problem

$$\mu = W u^{tr} G u / v^{tr} O v$$

(8)

with $W = \Delta^{N-1} \tau^{N-1} \epsilon^{N} / (\epsilon^N \Omega^{N-1} \tau_d^{N-1})$. Note that $\zeta$ is quadratically involved here, and therefore the maximization of $\mu$ gives a similar generalized eigenvalue problem as Eq(3).

$$E_{ptijkl} \equiv \eta_{ppqrstijkl} \tilde{B}_{ijkl} \eta_{ttk}$$

(9)

where $\mu = \tilde{\mu} W$. When the iteration is converged, the spontaneous magnetization and the internal energy in three dimension are calculated as, note the same formula Eq(3) and Eq(7) in two dimension,

$$M = u^{tr} \tilde{G} u / (\tilde{\mu} \tau_d)$$

(10)

FIG. 2: Spontaneous magnetization vs. temperature in two dimension. From right to left, the entanglement $p=1, 2 and 8$ (star, red online). The leftmost solid line (blue online) is the exact result of Yang [2].

FIG. 3: The same as Fig.2 for the specific heat. The peak is at $T = 2.278$. The thick solid line (blue online) is the exact result of Onsager [1].

$$E = -D u^{tr} \tilde{G}^2 u / (\tilde{\mu} \tau_d)$$

(11)

The results for the spontaneous magnetization and the specific heat in two dimension are shown in Fig.2 and 3. The results with the entanglement $p = 8$ are indistinguishable from the exact ones of Onsager and Yang. The obtained critical temperature 2.278 is 0.4% off the exact value 2.269185. The results in three dimension are shown.
FIG. 4: Spontaneous magnetization vs. temperature in three dimension. From right to left, the entanglement \((p,q) = (1,1), (1,2), (2,1), (2,2)\) and \((2,4)\) (star, red online), where \(p\) refers to the entanglement associated with \(\zeta\) and \(q\) with \(\xi\) and \(\eta\). For \(p=1\), the \((1,2)\) result is the converged one. The leftmost solid line (blue online) is the empirical formula from the RG-finite-size-scaling-MC method [10].

\[
M(t) = -t^{0.32694109}(1.6919045 - 0.34357731t^{0.50842026} - 0.42572366t), \tag{12}
\]

for \(0.0005 < t < 0.26\) where \(t = 1 - 0.2216544kT\). The obtained critical temperature 4.547 is 0.8% off the believed exact value 4.5114(1). The specific heat in three dimension has a marked difference from two dimension, namely it is highly asymmetric near the critical point. In fact our result with the entanglement \((2,4)\) has quite a resemblance to both the MC prediction [14] (also on page 479 of [15]) and the specific heat experiment on argon at the gas-liquid phase transition [16] (also on page 13 of [8]). It may be worth pointing out that the method can calculate equilibrium properties easily to a high precision. As is seen in Fig. 1-4, the \(p=2\) case in two dimension and the \((2,2)\) case in three dimension give fairly precise results, but it took only 30 minutes using a single PC of about 1GHz processing speed.

Because of simplicity and generality of the method, many applications and further progresses are anticipated, but from a theoretical viewpoint, the entanglement \(p = 3\) case in three dimension needs to be resolved first to see the swift convergence with the increase of entanglement. The simplest case \((3,1)\), however, was done easily giving at most (near the transition point) \(10^{-3}\) relative correction to the case \((2,1)\), indicating that the correction from \(p = 3\) will indeed be very small. After confirming this point, the method would serve as an exact method for most of the purposes in equilibrium statistical physics. As for a much more accurate analysis of the transition point such as \(T_c\) and various critical exponents beyond \(1\%\) level, as was done in [9–11, 17], it is interesting to see how a combination of RG and the present method performs.

In conclusion, the essence of the new method shall be summarized and further clarified. First, it is not a kind of cluster mean field theories or transfer-matrix mean field theories as used, e.g., in the coherent anomaly method [18]. In our word, the cluster mean field theories are described as the case with entanglement \(= 1\), but each \(\zeta\) there represents a cluster of bonds. By considering entanglement greater than \(1\), we go beyond mean field theories. Second, we have not made any assumptions, nor used any peculiar procedures only applicable to the Ising models. We have used SVD repeatedly and the key idea of our method is to fully implement the translational symmetry. Third, one might still press for an evidence of power of the new method. For that matter, we simply note that the new method has been successfully extended to the 1D Hubbard model, reproducing the main results of Bethe Ansatz [19]. Finally, a deep question is if our method offers a new physical concept or picture. For this, we point out that the state \(\varphi_0\) for the Hubbard model includes, as a special case, the resonating-valence-bond (RVB) state proposed by Anderson for the high-temperature superconductors [20]. We note that the resonating character of the Anderson wave function is a natural consequence of the translational symmetry. In this sense, our state \(\varphi_0\) is always resonating. It could be any states, superconduct-
ing, insulating, metallic or magnetic. Our method thus opens a possibility of precise determination of the phase diagram of the 2D Hubbard model. An effort toward this goal is currently under way, and will be reported in a future publication.

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