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Thermal Pure Quantum States at Finite Temperature

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An equilibrium state can be represented by a pure quantum state, which we call a thermal pure quantum (TPQ) state. We propose a new TPQ state and a simple method of obtaining it. A single realization of the TPQ state suffices for calculating all statistical-mechanical properties, including correlation functions and genuine thermodynamic variables, of a quantum system at finite temperature.

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The possibility of extracting statistical-mechanical information from a pure quantum state has been intensively discussed in the context of the foundation of statistical mechanics [1–4]. As we shall demonstrate here, it also has a potential significance for a new formulation of statistical mechanics, and for a novel calculation technique.

As an illustration, let us consider an isolated system composed of N spins. In the ensemble formulation, its equilibrium properties are described by the microcanonical ensemble, which is specified by E (energy), N, and so on. The corresponding subspace (energy shell) in the Hilbert space $\mathcal{H}_N$ is denoted by $\mathcal{E}_{E,N}$. Let us consider a random vector $|\psi\rangle = \sum_\nu' c_\nu |\nu\rangle$ in $\mathcal{E}_{E,N}$, where $\{|\nu\rangle\}_\nu$ is an arbitrary orthonormal basis set of $\mathcal{E}_{E,N}$, $\sum_\nu'$ denotes the sum over this basis, and $\{c_\nu\}_\nu$ is a set of random complex numbers drawn uniformly from the unit sphere $\sum_\nu' |c_\nu|^2 = 1$ in the complex space of dimension $\dim\mathcal{E}_{E,N}$. It was shown in Refs. [1–4] that almost every such vector gives the correct equilibrium values of a certain class of observables $\hat{A}$ by $\langle\psi|\hat{A}|\psi\rangle$. This property was proved in Refs. [1,2] for observables of a subsystem, which is much smaller than the whole system. The case of general observables, including observables of the whole system (such as the total magnetic moment and its fluctuation), was analyzed in Refs. [3,4]. It was shown that the above property holds not for all observables but for observables that are low-degree polynomials (i.e., their degree $\ll N$) of local operators [3]. We here call such observables mechanical variables. We assume that all mechanical variables are normalized as dimensionless.

For conceptual clarity, we call generally a pure quantum state that represents an equilibrium state a thermal pure quantum state. Stating more precisely for the case where a state $|\psi\rangle$ has random variables (such as the random vector discussed above), we call $|\psi\rangle$ a TPQ state if for an arbitrary positive number ϵ

$$\mathrm{P}\left(|\langle\psi|\hat{A}|\psi\rangle - \langle\hat{A}\rangle^{\mathrm{eq}}_{E,N}| \geq \epsilon\right) \leq \eta_\epsilon(N) \tag{1}$$

for every mechanical variable $\hat{A}$. Here, $\mathrm{P}(x)$ denotes the probability of event x, $\langle\cdot\rangle^{\mathrm{eq}}_{E,N}$ denotes the ensemble average, and $\eta_\epsilon(N)$ is a function (of N and ϵ) which vanishes as $N \to \infty$. Inequality (1) means that for large N getting a single realization of a TPQ state is sufficient, with high probability, for evaluating equilibrium values of mechanical variables. The vector $\sum_\nu' c_\nu|\nu\rangle$ of Refs. [1–4] is a TPQ state. However, genuine thermodynamic variables, such as the entropy and temperature, cannot be calculated as $\langle\psi|\hat{A}|\psi\rangle$ because they are not mechanical variables [5]. Moreover, such a TPQ state is practically hard to construct because a basis $\{|\nu\rangle\}_\nu$ of $\mathcal{E}_{E,N}$ is hard to obtain.

In this Letter, we propose a new TPQ state, a novel method of constructing it, and new formulas for obtaining genuine thermodynamic variables. This enables one to calculate all variables of statistical-mechanical interest at finite temperature, from only a single realization of the TPQ state. We also show that this novel formulation is very useful for practical calculations.

New TPQ state.—We consider a discrete quantum system composed of N sites, which is described by a Hilbert space $\mathcal{H}_N$ of dimension $D = \lambda^N$, where λ is a constant of $O(1)$. [For a spin 1/2 system, $\lambda = 2$.] Our primary purpose is to obtain results in the thermodynamic limit: $N \to \infty$ while E/N is fixed. Therefore, we hereafter use quantities per site, $\hat{h} \equiv \hat{H}/N$ (where $\hat{H}$ denotes the Hamiltonian), $u \equiv E/N$, and $(u; N)$ instead of (E, N). [We do not write explicitly variables other than u and N, such as a magnetic field.] We assume that the system is consistent with thermodynamics in the sense that the density of states $g(u; N)$ behaves as [6]

$$g(u;N) = \exp[Ns(u;N)], \qquad \beta'(u;N) \leq 0. \tag{2}$$

Here, $s(u;N)$ is the entropy density, which converges to the N independent one $s(u;\infty)$ as $N \to \infty$, $\beta(u;N) \equiv \partial s(u;N)/\partial u$ is the inverse temperature, and $\beta' \equiv \partial\beta/\partial u$. Since D is finite, β may be positive and negative in lower and higher energy regions, respectively. We here consider the former region.

We propose the following TPQ state and the procedure for constructing it. First, take a random vector $|\psi_0\rangle \equiv \sum_i c_i|i\rangle$ from the whole Hilbert space $\mathcal{H}_N$. Here, $\{|i\rangle\}_i$ is an arbitrary orthonormal basis of $\mathcal{H}_N$, and $\{c_i\}_i$ is a set of random complex numbers drawn uniformly from the unit sphere $\sum |c_i|^2 = 1$ of the D dimensional complex space. Note that this construction of a random vector is independent of the choice of the basis $\{|i\rangle\}_i$. One can therefore use a trivial basis such as a set of product states. Hence, $|\psi_0\rangle$ can be generated easily. On the whole, the amplitude is equally distributed over all the energy eigenstates in this state (as is easily seen by choosing the eigenstates of $\hat{h}$ as the basis $\{|i\rangle\}_i$). Thus, the distribution of energy in $|\psi_0\rangle$ is proportional to $g(u;N)$. We wish to modify this distribution into another distribution $r_k(u;N)$ which has a peak at a desired energy. This is easily done by operating a suitable polynomial of $\hat{h}$ onto $|\psi_0\rangle$ as we shall see below. We denote the minimum and the maximum eigenvalues of $\hat{h}$ by $e_{\min}$ and $e_{\max}$, respectively. Take a constant l of $O(1)$ such that $l \geq e_{\max}$. Starting from $|\psi_0\rangle$, calculate

$$u_k \equiv \langle \psi_k | \hat{h} | \psi_k \rangle, \tag{3}$$

$$|\psi_{k+1}\rangle \equiv (l - \hat{h})|\psi_k\rangle / \parallel (l - \hat{h})|\psi_k\rangle \parallel, \tag{4}$$

iteratively for $k = 0, 1, 2, \ldots$. From Eq. (7) below, u_0 corresponds to $\beta = 0$; i.e., $g(u;N)$ takes the maximum at $u = u_0$. We will also show that u_k decreases gradually down to $e_{\min}$ as k is increased, i.e., $u_0 > u_1 > \ldots \geq e_{\min}$. One may terminate the iteration when u_k gets low enough for one's purpose. We denote k at this point by k_{term}. We will show that $k_{\mathrm{term}} = O(N)$ at finite temperature, and that the states $|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_{k_{\mathrm{term}}}\rangle$ become a series of TPQ states corresponding to various energy densities, $u_0, u_1, \ldots, u_{k_{\mathrm{term}}}$. Hence, the equilibrium value of an arbitrary mechanical variable $\hat{A}$ is obtained as $\langle \psi_k | \hat{A} | \psi_k \rangle$, as a function of u_k. For each realization of $\{c_i\}_i$, a series of realizations of TPQ states is obtained. We will show that the dependence of $\langle \psi_k | \hat{A} | \psi_k \rangle$ on $\{c_i\}_i$ is exponentially small in size N as N increases. Therefore, only a single realization suffices for getting a fairly accurate value. When better accuracy is required, one can take the average over many realizations.

We now show that the states obtained with the above procedure are TPQ states. Since $|\psi_0\rangle$ is independent of the choice of the basis, we take the set of energy eigenstates $\{|n\rangle\}_n$ as $\{|i\rangle\}_i$ in order to see properties of $|\psi_k\rangle$ (although we never use such a basis in practical calculations). After k-times multiplication of $l - \hat{h}$, $|\psi_0\rangle = \sum_n c_n |n\rangle$ turns into

$$|\psi_k\rangle \propto (l - \hat{h})^k |\psi_0\rangle = \sum_n c_n (l - e_n)^k |n\rangle, \tag{5}$$

where $\hat{h}|n\rangle = e_n|n\rangle$. Let us examine how the energy density u distributes in this state. The (unnormalized) distribution function of u is given by $r_k(u;N) \equiv \delta_r^{-1} \sum_n'' |c_n|^2 (l - e_n)^{2k}$, where $\delta_r = o(1)$ and the sum is taken over n such that e_n lies in a small interval $[u - \delta_r/2,\ u + \delta_r/2)$. Since the density of states $g(u;N)$ is exponentially large in size N, $r_k(u;N)$ converges (in probability) exponentially fast to its average. Hence,

$$r_k(u;N) = D^{-1} \exp[N \xi_\kappa(u;N)], \tag{6}$$

where $\xi_\kappa(u;N) \equiv s(u;N) + 2\kappa \ln(l - u)$ with $\kappa \equiv k/N$. Hereafter, we often denote k dependence by κ; e.g., we express u_k as u_κ. Note that $\xi_\kappa(u;N)$ does not depend on $\{c_i\}_i$, because the dependence vanishes when we have dropped negligible terms in Eq. (6). $\xi_\kappa(u;N)$ takes the maximum at u_κ^* which satisfies

$$\beta(u_\kappa^*;N) = 2\kappa/(l - u_\kappa^*). \tag{7}$$

Since $\beta(u_\kappa^*;N)$ and $l - u_\kappa^*$ are $O(1)$, we find $\kappa = O(1)$, and hence $k = O(N)$. Expanding $\xi_\kappa(u;N)$ around u_κ^*, and noticing $\xi_\kappa'' \equiv \partial^2 \xi_\kappa / \partial u^2 = \beta'(u_\kappa^*;N) - 2\kappa/(l - u_\kappa^*)^2 < 0$ from Eq. (2), we get $\xi_\kappa(u;N) = \xi_\kappa(u_\kappa^*;N) - |\xi_\kappa''|(u - u_\kappa^*)^2/2 + \xi_\kappa'''(u - u_\kappa^*)^3/6 + \ldots$. Here, $\xi_\kappa''' \equiv \partial^3 \xi_\kappa / \partial u^3 = \beta''(u_\kappa^*;N) - 4\kappa/(l - u_\kappa^*)^3$. Hence, $r_k(u;N)$ behaves almost as the Gaussian distribution, peaking at $u = u_\kappa^*$, with the vanishingly small variance $1/N|\xi_\kappa''|$. Let us introduce the density operator $\hat{\rho}_k \equiv (l - \hat{h})^{2k} / \mathrm{Tr}(l - \hat{h})^{2k}$, which has the same energy distribution $r_k(u;N)$. In the ensemble formulation, $\hat{\rho}_k$ represents the equilibrium state specified by $(u_\kappa;N)$ because $r_k(u;N)$ has a sharp peak. We call the ensemble corresponding to $\hat{\rho}_k$ the smooth microcanonical ensemble (because the energy distribution is smooth). In a way similar to those of Refs. [3,4], we can show that for an arbitrary positive number ϵ

$$\mathrm{P}(|\langle \psi_k | \hat{A} | \psi_k \rangle - \mathrm{Tr}[\hat{\rho}_k \hat{A}]| \geq \epsilon) \leq \frac{\|\hat{A}\|^2 r_k(e_{\min};N)}{\epsilon^2 r_k(u_\kappa^*;N)}, \tag{8}$$

$$\overline{\langle \psi_k | \hat{A} | \psi_k \rangle} = \mathrm{Tr}[\hat{\rho}_k \hat{A}], \tag{9}$$

for every mechanical variable $\hat{A}$. Here, $\|\cdot\|$ denotes the operator norm [7], and the overline represents the random average. With increasing N, $\|\hat{A}\|^2$ grows at most as a low-degree polynomial of N, whereas $r_k(e_{\min};N)/r_k(u_\kappa^*;N)$ decreases exponentially at finite temperature (i.e., for $u_\kappa^* > e_{\min}$). Therefore, $|\psi_k\rangle$ is a TPQ state for the smooth microcanonical ensemble.

Genuine thermodynamic variables.—One might think it impossible to obtain genuine thermodynamic variables by only manipulating pure quantum states. However, our new TPQ state makes it possible. In fact, by substituting u_κ for u_κ^* in Eq. (7), and using Eq. (11) below, we obtain

$$\beta(u_\kappa;N) = 2\kappa/(l - u_\kappa) + O(1/N). \tag{10}$$

This gives $\beta(u_\kappa;N)$, with an error of $O(1/N)$, as a function of u_κ [because κ and l are known parameters]. That is, one obtains the temperature of the equilibrium state specified by $(u_\kappa;N)$ just by calculating u_κ with Eq. (3).

We can also obtain formulas with less errors. Using Eq. (6) and the expansion of $\xi_\kappa(u;N)$, we have

$$u_\kappa^* = u_\kappa^\bullet + O(1/N^2), \qquad u_\kappa^\bullet \equiv u_\kappa - \xi_\kappa'''/2N\xi_\kappa''^2. \tag{11}$$

Substituting $u_\kappa^\bullet$ for u_κ^* in Eq. (7), we get a better formula

$$\beta(u_\kappa^\bullet;N) = 2\kappa/(l - u_\kappa^\bullet) + O(1/N^2). \tag{12}$$

One can evaluate ξ''_κ and ξ'''_κ easily by calculating $\langle \psi_k|(\hat{h} - u_\kappa)^2|\psi_k\rangle = 1/N|\xi''_\kappa| + O(1/N^2)$ and $\langle \psi_k|(\hat{h}-u_\kappa)^3|\psi_k\rangle = \xi'''_\kappa/N^2|\xi''_\kappa|^3 + O(1/N^3)$. Hence, using formula (12), one obtains $\beta(u;N)$ (for $u = u_0^\bullet, u_1^\bullet, \ldots$) with an error of $O(1/N^2)$. In a similar manner, we can obtain formulas whose errors are of even higher order of $1/N$.

However, $\beta(u;N)$ is the inverse temperature of a finite system, whereas we are most interested in its thermodynamic limit $\beta(u;\infty)$. In general, the difference $|\beta(u;N) - \beta(u;\infty)|$ decays not so quickly as $O(1/N^2)$. To obtain a better formula for $\beta(u;\infty)$, we consider C identical copies of the N-site system. We denote quantities of this CN-site system by tilde, such as $|\tilde{\psi}_0\rangle \equiv |\psi_0\rangle^{\otimes C}$. The state $|\tilde{\psi}_{\tilde{k}}\rangle$ is given by $|\tilde{\psi}_{\tilde{k}}\rangle \propto (\tilde{l} - \tilde{h})^{C\tilde{k}}|\tilde{\psi}_0\rangle$, where $\tilde{h} \equiv (\hat{H} \otimes \hat{1}^{\otimes(C-1)} + \hat{1} \otimes \hat{H} \otimes \hat{1}^{\otimes(C-2)} + \cdots + \hat{1}^{\otimes(C-1)} \otimes \hat{H})/CN$. In the limit of $C \to \infty$, $\tilde{u}_{\tilde{\kappa}}$ approaches the canonical average of u in a single copy with inverse temperature $\tilde{\beta}(\tilde{u}_{\tilde{\kappa}};\infty)$. At the point where $\tilde{\beta}(\tilde{u}_{\tilde{\kappa}};\infty) = \beta(u^*_\kappa;N)$ is satisfied, we can estimate this canonical average, which is denoted by $\tilde{u}^{\mathrm{c}}_\kappa$, in the same manner as Eq. (11). Then, we get $\tilde{u}^{\mathrm{c}}_\kappa = \tilde{u}^\bullet_\kappa + O(1/N^2)$, where

$$\tilde{u}^\bullet_\kappa \equiv u^\bullet_\kappa + \frac{\xi'''_\kappa + 4\kappa/(l - u^\bullet_\kappa)^3}{2N[\xi''_\kappa + 2\kappa/(l - u^\bullet_\kappa)^2]^2}. \tag{13}$$

We thus find

$$\tilde{\beta}(\tilde{u}^\bullet_\kappa;\infty) = 2\kappa/(l - u^\bullet_\kappa) + O(1/N^2), \tag{14}$$

which gives the inverse temperature $\tilde{\beta}(u;\infty)$ (for $u = \tilde{u}^\bullet_0, \tilde{u}^\bullet_1, \ldots$) of an infinite system composed of an infinite number of N-site systems. We expect that $\tilde{\beta}(u;\infty)$ is much closer to $\beta(u;\infty)$ than $\beta(u;N)$, because information of $\xi(u;N)$ in the whole spectrum range of u is included in $\tilde{\beta}(u;\infty)$. [By contrast, only the information at the peak of $\xi(u;N)$ is included in $\beta(u;N)$.] This will be confirmed later by numerical computation.

We can also obtain the entropy density s as a function of u and h_z, by integrating β over u and βm_z over h_z [8]. For example, for an arbitrarily fixed value of h_z, we have $s(u_{2p}) - s(u_{2q}) = \sum_{\ell=p}^{q-1} v(u^\bullet_{2\ell}, u^\bullet_{2\ell+1}, u^\bullet_{2\ell+2}) + O(1/N^2)$ by generalizing Simpson's rule. Here, u stands for $(u;\ N)$ or $(u;\ \infty)$, p and q are integers, and $v(x,y,z) \equiv (x-z)\{\beta(x)+\beta(z)\}/2-(x-z)^2[x\{\beta(z)-\beta(y)\}+y\{\beta(x)-\beta(z)\}+z\{\beta(y)-\beta(x)\}]/6(x-y)(y-z)$.

To sum up, we have established a new formulation of statistical mechanics, whose fundamental formulas are Eqs. (5) and (10) [9].

Numerical results.—Our formulation is easily implemented as a method of numerical computation. We apply it to the one-dimensional Heisenberg model in order to confirm the validity of the formulation. We take $\hat{H} = \frac{J}{4}\sum_{i=1}^N[\hat{\boldsymbol{\sigma}}(i) \cdot \hat{\boldsymbol{\sigma}}(i+1) - h_z\hat{\sigma}_z(i)]$, where $J = -1$ (ferromagnetic) or $+1$ (antiferromagnetic). For $N \to \infty$, the exact results at finite temperature (i.e., $u > e_{\mathrm{min}}$) have been derived for magnetization $m_z \equiv N^{-1}\sum_{i=1}^N\langle\sigma_z(i)\rangle^{\mathrm{eq}}_{u;N}$ [10], and for the correlation function $\phi(j) \equiv N^{-1}\sum_{i=1}^N\langle\sigma_z(i)\sigma_z(i+j)\rangle^{\mathrm{eq}}_{u;N}$ [11]. They are plotted in Figs. 1 and 2 by solid lines, where different lines correspond to different values of u. We calculate the corresponding results using our formulation. The results for $N = 24$ are plotted by circles [12], where each circle is obtained from a single realization of TPQ state. According to Eq. (8), choice of the initial random numbers $\{c_i\}_i$ has only an exponentially small effect on the results at finite temperature. We have confirmed this fact by observing that the standard deviation, computed from ten realizations of a TPQ state for each data point, is smaller than the radius of the circles of these figures. Results for other values of N are plotted in Fig. 1 for $u = -0.3J$, and in the left insets of Fig. 2. It is seen that the N dependence becomes fairly weak for $N \gtrsim 20$, and that the results for $N = 24$ agree well with the exact results. As illustrated by this example, N should be increased in our method until the variation of the results with increasing N becomes less than the required accuracy.

We have also computed $\phi(j)$ at finite h_z and T, for which exact results are unknown. The results at $T \simeq 0.45J$ are plotted in the right inset of Fig. 2.

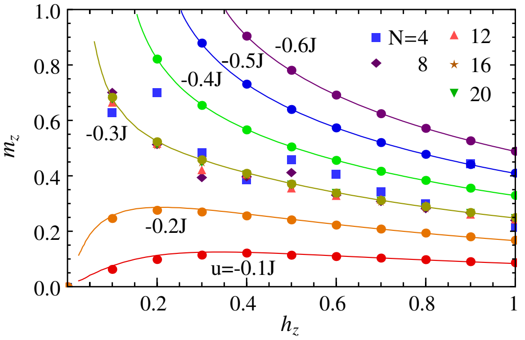

FIG. 1 (color online). m_z vs h_z for $J = -1$. Solid lines: exact results for $N \to \infty$, for various values of u [10]. Circles: results of our formulation for $N = 24$. Results for $N = 4$–20 are also shown for $u = -0.3J$.

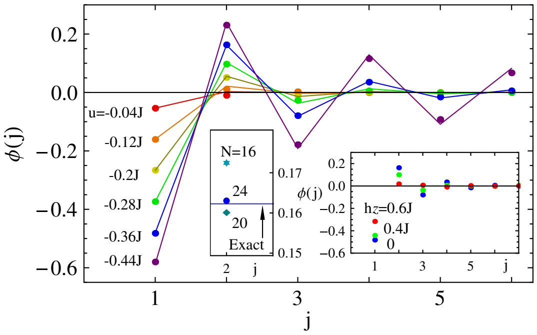

FIG. 2 (color online). $\phi(j)$ for $J = +1$ and $h_z = 0$. Solid lines: exact results for $N \to \infty$, for various values of u [11]. Circles: results of our formulation for $N = 24$. (left inset) Results for $N = 16$–24 at $j = 2$ for $u = -0.36J$. (right inset) $\phi(j)$ at finite h_z, obtained from a single realization of the TPQ state at $T \simeq 0.45J$.

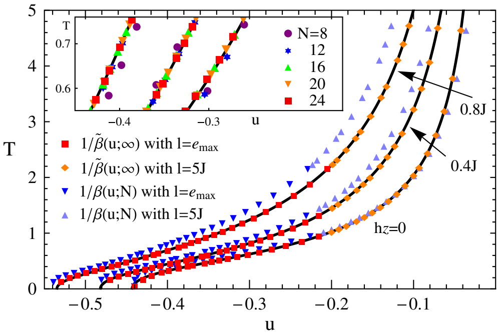

FIG. 3 (color online). T vs u for $J = +1$. Solid lines: exact results for $N \to \infty$, for $h_z = 0 - 0.8J$ [13]. Triangles and squares: our results for $\beta^{-1}(u;N)$ (triangles) and $\tilde{\beta}^{-1}(u;\infty)$ (squares) for $N = 24$. (inset) $\tilde{\beta}^{-1}(u;\infty)$ for $N = 8$–24.

For genuine thermodynamic variables, the exact result for $1/\beta(u;\infty)$ [13] is plotted by solid lines in Fig. 3. Corresponding results for $1/\beta(u;N)$ and $1/\tilde{\beta}(u;\infty)$, obtained with our method with $N = 24$, are plotted by triangles and squares, respectively, where each point is obtained from a single realization of the TPQ state. [We have confirmed again that dependence on the choice of $\{c_i\}_i$ is negligibly small.] Not only $\beta(u;N)$ but also $\tilde{\beta}(u;\infty)$ depend on N. However, the dependence of $\tilde{\beta}(u;\infty)$ becomes fairly weak for $N \gtrsim 20$, as shown in the inset. $\tilde{\beta}(u;\infty)$ for $N = 24$ agrees well with the exact result, whereas $\beta(u;N)$ differs significantly from them for this value of N. We have thus confirmed that $\tilde{\beta}(u;\infty)$ is much closer to $\beta(u;\infty)$ than $\beta(u;N)$, for finite N. Note, however, that $\beta(u;N)$ gives almost correct result for β of a finite system, as seen from Eq. (12).

We have obtained a series of TPQ states at the discrete points $u_0, u_1, u_2, \ldots, u_{\text{term}}$, whose intervals are $O(1/N)$, vanishing as $N \to \infty$. For each value of N, Eq. (7) shows that k gets smaller for smaller l to reach the same u and T, increasing the intervals and reducing the amount of computation. We have taken $l \simeq e_{\max}$ in Figs. 1 and 2. In Fig. 3, we have performed computations with $l = e_{\max}$ and $5J$, and both results agree well with each other.

Advantages.—When applied to numerical computation, our formulation has the following advantages. At finite T, an exponentially large number of states are included in $\mathcal{E}_{E,N}$. This makes conventional methods pretty hard. In contrast, our method takes full advantage of such a huge number of states, as seen, e.g., in the derivation of Eq. (6). Moreover, our method is applicable to systems of any spatial dimensions, and to frustrated or fermion systems as well. Furthermore, our method costs much less computational resources than the numerical diagonalization. For example, the number of non-vanishing elements of $\hat{H}$ of the Heisenberg model is $O(N2^N)$. Since $k = O(N)$, the computational time is $O(N^2 2^N)$, which is exponentially shorter than that of diagonalization. In fact, it took only two hours to compute all data in Fig. 3 on a personal computer. Computations can be made even faster by parallelizing the algorithm, which is quite easy and efficient because our method consists only of matrix multiplications. Furthermore, our method is effective over a wide range of T because the rhs of Eq. (8) is exponentially small as long as s (and hence T) is finite of $O(1)$. In fact, Figs. 1–3 show that our results agree well with the rigorous results in a wide range of T, from $T \ll J$ to $T \gg J$. In practical computations with finite N, $T\ (= 1/\tilde{\beta}(u_\kappa^\bullet;\infty))$ can be lowered as long as $r_k(e_{\min};N)/r_k(u_\kappa^*;N) \ll 1$. We expect that our method will make it possible to analyze systems which could not be analyzed with other methods.

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[5] Entropy could be obtained if one could obtain a TPQ state of a huge system which includes the target system. However, this is harder than calculating the partition function.

[6] These are the conditions that the Boltzmann formula gives the correct thermodynamic entropy and that the system is stable. Hence, they are necessary for all microscopic models to which statistical mechanics is applied.

[7] When $\hat{A}$ is unbounded, $\|\hat{A}\|$ should be replaced with $\max_{|\phi\rangle \in \mathcal{H}_N^{\subseteq}} |\langle\phi|\hat{A}|\phi\rangle|$, where $\mathcal{H}_N^{\subseteq}$ denotes a Hilbert subspace in which the values of macroscopic variables (such as u and m_z) are limited to certain finite ranges.

[8] We have also developed another method of obtaining s, in which $g(u;N)$ is directly evaluated from the inner products among different realizations of a TPQ state [S. Sugiura and A. Shimizu, Proc. Meeting of Phys. Soc. Jpn. 2011, paper number 23aGA-6].

[9] We can generalize Eq. (5) as $|\psi\rangle \propto Q(\hat{h})|\psi_0\rangle$. Here, $Q(u)$ is any differentiable real function such that $Q(u)^2 g(u;N)$ has a sharp peak, whose width and tails vanish as $N \to \infty$. This defines other new TPQ states, for which Eq. (7) is replaced with $\beta(u^*;N) + 2Q'(u^*)/NQ(u^*) = 0$.

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[12] One can evaluate the magnetic susceptibility $(\partial m_z/\partial h_z)_u$ and $(\partial m_z/\partial h_z)_T$ from Figs. 1–3.

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