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 a closed quantum system composed of $N$ spins, which is enclosed by adiabatic walls. 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 $\{|\nu\rangle\}$ is an arbitrary orthonormal basis set of $\mathcal{E}_{E,N}$, $\sum_{\nu}|c_{\nu}|^2 = 1$ in the complex space of dimension $\text{dim}\mathcal{E}_{E,N}$. It was shown in Refs. [1–4] that almost every such vector gives the correct equilibrium values of a certain class of observables $A$ by $\langle\psi|A|\psi\rangle$. 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. We here call such observables mechanical variables. We assume that all mechanical variables are normalized in such a way that they are dimensionless.

For conceptual clarity, we call generally a pure quantum state that represents an equilibrium state a thermal pure quantum state (TPQ 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 $\epsilon$

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

for every mechanical variable $A$. Here, $P(x)$ denotes the probability of event $x$, $\langle\cdot\rangle^\text{eq}_{E,N}$ denotes the ensemble average, and $\eta_e(N)$ is a function (of $N$ and $\epsilon$) which vanishes as $N \to \infty$. The above inequality 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, important problems remain to be solved. Most crucially, genuine thermodynamic variables, such as the entropy and temperature, cannot be calculated as $\langle\psi|A|\psi\rangle$ because they are not mechanical variables. Moreover, one needs to prepare a basis $\{|\nu\rangle\}$ of $\mathcal{E}_{E,N}$ to construct $\sum_{\nu} c_{\nu}|\nu\rangle$. Since this is a hard task, such a TPQ state is hard to obtain.

In this Letter, we resolve these problems by proposing a new TPQ state, a novel method of constructing it, and new formulas for obtaining genuine thermodynamic variables. This novel formulation of statistical mechanics 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 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 $\lambda$ 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, $\Bar{h} \equiv \Bar{H}/N$ (where $\Bar{H}$ denotes the Hamiltonian), $\Bar{u} \equiv E/N$, and $\Bar{u} = \langle u\rangle$ 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

$$g(u; N) = \exp[N s(u; N)], \quad \beta'(u; N) \leq 0.$$ (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 $\beta' \equiv \partial \beta/\partial u$. These conditions are satisfied, for example, by spin models and the Hubbard model. Since $D$ is finite, $\beta$ 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\}, 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 random vectors is independent of the choice of the orthonormal 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 other hand, the amplitude is almost 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\}). Thus, the distribution of energy in $|\psi_0\rangle$ is proportional to $g(\hat{n}; N)$. We wish to modify this distribution into another distribution $r_k(\hat{n}; N)$ which has a peak at an desired energy. This is easily done by operating a suitable polynomial of $\hat{h}$ onto $|\psi_0\rangle$ as we shall see below. 

[Operating $\hat{h}$ onto a vector is much easier than diagonalizing $\hat{h}$.] We denote the minimum and the maximum eigenvalues of $\hat{h}$ by $e_{\text{min}}$ and $e_{\text{max}}$, respectively. Take a constant $l$ of $O(1)$ such that $l \geq e_{\text{max}}$. Starting from $|\psi_0\rangle$, calculate

$$u_k = \langle \psi_k | \hat{h} | \psi_k \rangle,$$

and

$$|\psi_{k+1}\rangle = (l - \hat{h})|\psi_k\rangle/||l - \hat{h}|\psi_k\rangle||$$

iteratively for $k = 0, 1, 2, \ldots$. From Eq. (6) below, $u_0$ corresponds to $\beta = 0$, i.e., $g(\hat{n}; N)$ takes the maximum at $u = u_0$. We will also show that $u_k$ decreases gradually down to $e_{\text{min}}$ as $k$ is increased, i.e., $u_0 > u_1 > \ldots > e_{\text{min}}$. One may terminate the iteration when $u_k$ gets low enough for one’s purpose. We denote $k$ at this point by $k_{\text{term}}$. We will show that $k_{\text{term}} = O(N)$ at finite temperature, and that the states $|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_{k_{\text{term}}}\rangle$ become a series of TPQ states corresponding to various energy eigenvalues, $u_0, u_1, \ldots, u_{k_{\text{term}}}$. 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\}, in order to see properties of $|\psi_k\rangle$ (although we never use such a basis in practical calculations). After $k$-times multiplication of $\hat{h}$, $|\psi_0\rangle = \sum_n c_n |n\rangle$ turns into

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

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 $r_k(u; N) \equiv \delta^{-1} \sum_n |c_n|^2 (l - e_n)^2$, where $\delta = O(1)$ and the sum is taken over $n$ such that $e_n$ lies in a small interval $[u - \delta/n, u + \delta/n]$. 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,

$$r_k(u; N) = D^{-1} \exp[N \xi_k(u; N)],$$

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

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

Since $\beta(u_{\kappa}^*; N)$ and $l - u_{\kappa}^*$ are $O(1)$, we find $\kappa = O(1)$, and hence $k = O(N)$. Expanding $\xi_k(u; N)$ around $u_{\kappa}^*$, and noticing

$$\xi'' \equiv \partial^2 \xi_k/\partial u^2 = \beta''(u_{\kappa}^*; N) - 2\kappa/(l - u_{\kappa}^*)^3 < 0$$

from Eq. (6), we get $\xi_k(u; N) = \xi_k(u_{\kappa}^*; N) - \xi''(u - u_{\kappa}^*)^3/6 + \cdots$. Here, $\xi'' \equiv \partial^3 \xi_k/\partial u^3 = \beta''(u_{\kappa}^*; N) - 4\kappa/(l - u_{\kappa}^*)^3$. Hence, $r_k(u; N)$ behaves almost as the Gaussian distribution, peaking at $u = u_{\kappa}^*$, with the vanishingly small variance $1/N|\xi''|$. Let us introduce the density operator $\tilde{\rho}_k \equiv (l - \hat{h})^{2k}/Tr(l - \hat{h})^{2k}$, which has the same energy distribution $r_k(u; N)$. In the ensemble formulation, $\tilde{\rho}_k$ represents the equilibrium state specified by $(u_{\kappa}; N)$ because $r_k(u; N)$ has a sharp peak. We call the ensemble corresponding to $\tilde{\rho}_k$ 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 $\epsilon$

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

for every mechanical variable $\hat{A}$. Here, $\|\cdot\|$ denotes the operator norm [5], and the overline represents the random average. With increasing $N$, $\|\hat{A}\|^2$ grows at most as a low-degree polynomial of $N$, whereas $r_k(e_{\text{min}}; N)/r_k(u_{\kappa}^*; N)$ decreases exponentially at finite temperature (i.e., for $u_{\kappa}^* > e_{\text{min}}$). 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 like the temperature and entropy by only manipulating pure quantum states. However, our new TPQ state makes it possible. In fact, by substituting $u_\kappa$ for $u_{\kappa}^*$ in Eq. (7), and using Eq. (11) below, we obtain

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

This gives $\beta(u_\kappa; N)$, with an error of $O(1/N)$, as a function of $u_\kappa$ [because $\kappa$ and $l$ are known parameters]. That
is, one obtains the temperature of the equilibrium state specified by \((u; N)\) just by calculating \(u^*_c\) with Eq. (9).

We can also obtain formulas with less errors. For example, using Eq. (8) and the expansion of \(\xi_N(u; N)\), we have

$$u^*_c = u^*_c + O(1/N^2), \quad u^*_c = u^*_c - \xi'''/2N\xi''^2.$$  \hspace{1cm} (11)

Substituting \(u^*_c\) for \(u^*_c\) in Eq. (10), we get a better formula

$$\beta(u^*_c; N) = 2\kappa/(l - u^*_c) + O(1/N^2).$$  \hspace{1cm} (12)

One can evaluate \(\xi'''\) and \(\xi''\) easily by calculating \(\langle \psi_k | (h - u^*_c)^2 | \psi_k \rangle = 1/N|\xi'''_N| + O(1/N^2)\) and \(\langle \psi_k | (h - u^*_c)^3 | \psi_k \rangle = \xi''''/N^2|\xi''_N|^3 + O(1/N^3)\). Hence, using formula (12), one obtains \(\beta(u; N)\) for \(u = u^*_c, u^*_c, \cdots\) 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 an even 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 \(\tilde{\psi}_0 \equiv |\psi_0\rangle \otimes \cdots \otimes |\psi_0\rangle\). The state \(|\tilde{\psi}_k\rangle\) is given by \(\langle \tilde{\psi}_k | \tilde{H} = (\tilde{h} - u^*_c)^2 | \tilde{\psi}_k \rangle = 1/N|\tilde{\psi}_k\rangle + O(1/N^2)\) and \(\langle \tilde{\psi}_k | (\tilde{h} - u^*_c)^3 | \tilde{\psi}_k \rangle = \tilde{\xi''''}/N^2|\tilde{\psi}_k\rangle^3 + O(1/N^3)\). Hence, using formula (12), one obtains \(\tilde{\beta}(u; N)\) for \(u = u^*_c, u^*_c, \cdots\) with an error of \(O(1/N^2)\). In the limit of \(C \rightarrow \infty\), \(\tilde{\beta}(u; \infty)\) approaches the canonical average of \(u\) in a single copy with inverse temperature \(\beta(u^*_c; \infty)\). At the point where \(\beta(u^*_c; \infty) = \beta(u^*_c; N)\) is satisfied, we can estimate this canonical average, which is denoted by \(\tilde{u}^*_c\), in the same manner as Eq. (11). Then, we get \(\tilde{u}^*_c = u^*_c + O(1/N^2)\), where

$$\tilde{u}^*_c = u^*_c + \frac{\xi'''}{2N|\xi''_N|^2} \langle \tilde{h} - u^*_c \rangle.$$  \hspace{1cm} (13)

We thus find

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

which gives the inverse temperature \(\tilde{\beta}(u; \infty)\) (for \(u = u^*_c, \tilde{u}^*_c, \cdots\)) 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 \(\beta(u; \infty)\). [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 \(\beta\) over \(u\) and \(\beta m_z\) over \(h_z\). For example, for an arbitrarily fixed value of \(h_z\), we have

$$s(u_{2p}) - s(u_{2q}) = \sum_{\ell = p}^{q-1} v(u_{2\ell}, u_{2\ell+1}, u_{2\ell+2}) + O(1/N^2).$$  \hspace{1cm} (15)

by generalizing Simpson’s rule. Here, \(u\) stands for \((u; N)\) or \((u; \infty)\), \(p\) and \(q\) are integers, and \(v(x, y, z) = (x - z)(y + z)/2 - (x - z)^2/2\{x\{y - \beta(x)\} + y\{\beta(x) - \beta(y)\}\} + 4\{\beta(x) - z\{y - \beta(x)\}\} + 6(x - y)(y - z)\). 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.

To sum up, one can obtain a series of TPQ states and values of all variables of statistical-mechanical interest, by preparing a random vector and simply applying \((l - \tilde{h})\) iteratively. That is, we have established a new formulation of statistical mechanics, whose fundamental formulas are Eqs. (5) and (15).

**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 \(\tilde{H} = \sum_{\ell = 1}^{N} |(i)\rangle\langle (i)| - h_z (\sigma_z (i))\), in which \(J = -1\) (ferromagnetic) or +1 (antiferromagnetic). For \(N \rightarrow \infty\), the exact results at finite temperature (i.e., \(\beta > \beta_{\text{min}}\)) have been derived for magnetization \(m_z \equiv \sum_{\ell = 1}^{N} \langle \sigma_z (i) \rangle_{\text{eq}}\) at all values of \(u\) and \(h_z\). [For correlation function \(\phi(j) = \sum_{\ell = 1}^{N} \langle \sigma_z (i) \sigma_z (i + j) \rangle_{\text{eq}}\) at all values of \(u\) with \(h_z = 0\).] They are plotted in Figs. 4 and 2 by solid lines, where different colors correspond to different values of \(u\). We calculate the corresponding results using our formulation, by performing numerical computation. The results for \(N = 24\) are plotted by circles, where each circle is obtained from a single realization of TPQ state. According to Eq. (5), choice of the initial random numbers \(\{\epsilon_i\}\), 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. 44 for \(u = -0.3J\), and in the left insets of Fig. 2 for \(u = -0.36J\) at \(j = 2\). 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 $T \approx 0.45J$ are plotted in the right inset of Fig. 2.

For genuine thermodynamic variables, the exact result for $1/\beta(u; \infty)$ is plotted by solid lines in Fig. 3. Corresponding results for $1/\beta(u; N)$ and $1/\beta(u; \infty)$, 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 at $T \approx 0.45J$.

Advantages — We now discuss advantages of our formulation when used as a method of numerical calculation. At finite $T$, an exponentially large number of states are included in $\hat{\mathcal{E}}_{E,N}$. This makes computation of eigenstates in $\hat{\mathcal{E}}_{E,N}$ 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. (4). As a result, using just a single realization of TPQ state, one can calculate all quantities of statistical-mechanical interest at finite $T$, on the solid theoretical basis that is developed in this Letter. 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 $O(N^2N)$. Since $k = O(N)$, the computational time is $O(N^2N)$ in our method, which is exponentially shorter than that of diagonalization. In fact, it took only two hours to compute all data in Fig. 3 on a PC. 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. (3) is exponentially small as long as $s$ (and hence $T$) is finite of $O(1)$. In fact, Figs. 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 \( N, T (= 1/\beta(u^*; \infty)) \) can be lowered as long as \( r_k(e_{\min}; N)/r_k(u^*; N) \ll 1 \).

We note that the quantum Monte Carlo method may be much faster. However, it suffers from the sign problem in frustrated systems and fermion systems. The density-matrix renormalization group method has been extended to finite temperature, and the state obtained in Ref. [15] might be close to TPQ states. However, its effectiveness in two- or more-dimensional systems is not clear yet. The states obtained with the microcanonical Lanczos method [16], which tried to obtain not TPQ states but eigenstates obtained with the microcanonical Lanczos method in two- or more-dimensional systems is not clear yet. The density to finite temperature, and the state obtained in Ref. [15] remains to be a TPQ state after making several remarks. First, one can evaluate the magnetization (i.e., decomposition into macroscopically definite states) by applying the variance-covariance matrix method of Ref. [13] to a TPQ state.

Fourth, Eq. (5) can be generalized as \(|\psi\rangle \propto Q(\hat{h})(|\psi\rangle)\), which defines other new TPQ states. Here, \( Q(u) \) is any differentiable real function such that \( Q(u)^2 g(u; N) \) has a sharp peak, whose width vanishes as \( N \to \infty \), and \( Q(u)^2 g(u; N) \) outside the peak decays quickly. Using this \(|\psi\rangle\), one can calculate various quantities as we have done using \(|\psi\rangle\). For instance, the formula corresponding to Eq. (7) is given by \( \beta(u^*; N) + 2Q(u^*)/NQ(u^*); Q(u) = 0 \).

Finally, although a TPQ state (such as \(|\psi\rangle\)) and the mixed state (such as \( \tilde{\rho}_k \)) of the corresponding ensemble are identical with respect to mechanical variables, they are completely different with respect to entanglement. At \( T \gg J \), for example, \( \tilde{\rho}_k \) has only small entanglement (because it is close to the completely mixed state \((1/D) I\), which has no entanglement), whereas we can show that \(|\psi\rangle\) has exponentially large entanglement (as previously shown for \( T \to \infty \) in Ref. [14]). It is thus seen that an equilibrium state can be represented either by a TPQ state with huge entanglement or by a mixed state with much less entanglement. Their difference can be detected only by high-order polynomials of local operators, which are not of statistical-mechanical interest [3,14].

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6. [4] A. Sugita and A. Shimizu, J. Phys. Soc. Jpn. 77, 106404 (2007).
7. [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.
8. [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.
