Thermal Pure Quantum States of Many-Particle Systems

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We generalize the thermal pure quantum (TPQ) formulation of statistical mechanics, in such a way that it is applicable to systems whose Hilbert space is infinite dimensional. Assuming particle systems, we construct the grand-canonical TPQ (gTPQ) state, which is the counterpart of the grand-canonical Gibbs state of the ensemble formulation. A single realization of the gTPQ state gives all quantities of statistical-mechanical interest, with exponentially small probability of error. This formulation not only sheds new light on quantum statistical mechanics but also is useful for practical computations. As an illustration, we apply it to the Hubbard model, on a one-dimensional (1d) chain and on a two-dimensional (2d) triangular lattice. For the 1d chain, our results agree well with the exact solutions over wide ranges of temperature, chemical potential and the on-site interaction. For the 2d triangular lattice, for which exact results are unknown, we obtain reliable results over a wide range of temperature. We also find that finite-size effects are much smaller in the gTPQ state than in the canonical TPQ (cTPQ) state. This also shows that in the ensemble formulation the grand-canonical Gibbs state of a finite-size system simulates an infinite system much better than the canonical Gibbs state.

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Quantum statistical mechanics has conventionally been formulated as the ensemble formulation, in which an equilibrium state is given by a mixed quantum state (Gibbs state) that is represented by a density operator $\hat{\rho}^{\text{ens}}$. Recently, another formulation, called the TPQ formulation, has been developed by two of the authors [1, 2], by generalizing theories of typicality [3–8]. In this formulation, an equilibrium state is given by a pure quantum state, which is called a TPQ state. Since the TPQ state is not a purification $\rho$ of $\hat{\rho}^{\text{ens}}$, it is totally different from $\hat{\rho}^{\text{ens}}$. In fact, the magnitudes of their entanglement are almost maximally different [10, 11]. Nevertheless, one can correctly obtain all quantities of statistical-mechanical interest, including thermodynamic functions, from a single state vector of a TPQ state [1, 2]. Because of this striking property, the TPQ formulation is very useful in practical applications [1, 2]. In fact, it has solved problems that are hard with conventional methods, such as the specific heat of a 2d frustrated spin system [2].

However, it was formulated only for systems whose Hilbert space $\mathcal{H}$ is finite dimensional. Since $\dim \mathcal{H} = \infty$ for many physical systems, such as particles in continuous space, generalization of the TPQ formulation is necessary. Furthermore, only the microcanonical TPQ (mTPQ) and cTPQ states were constructed, and their validity was confirmed separately [1, 2]. Although all TPQ states give the same results in the thermodynamic limit [2], they will give different results for finite-size systems because of finite-size effects. To study infinite systems, it is desirable to develop other TPQ states (such as the gTPQ state) and to clarify which TPQ state of finite size gives results closest to those of infinite systems.

In this Rapid Communication, we generalize the TPQ formulation so that it will be applicable to the case where $\dim \mathcal{H}$ and the norm of operators (such as the momentum) are infinite. Assuming particle systems as a concrete example, we construct the gTPQ state, which are specified by inverse temperature $\beta = 1/T$, chemical potential $\mu$, volume $V$, magnetic field $h$, and so on. [In the following, we abbreviate $\beta, \mu, V, h, \ldots$ simply as $\beta, \mu, V$.]

We show that a single realization of the gTPQ state gives all quantities of statistical-mechanical interest, including thermodynamic functions. This striking property is not only interesting as a fundamental physics, but also useful for practical computations, because it enables one to solve problems that are hardly solvable by other methods. As an illustration, we apply the TPQ formulation to numerical studies of the Hubbard model, on a 1d chain and on a 2d triangular lattice. We obtain reliable results, over wide ranges of $T, \mu$ and the on-site interaction $U$. Moreover, we show that as compared with the cTPQ state with finite $V$ the gTPQ state with the same $V$ gives results much closer to the exact results for an infinite system. The same can be said for the canonical and grand-canonical Gibbs states of the ensemble formulation.

Mechanical variables – Statistical mechanics treats ‘mechanical variables’, such as energy, and ‘genuine thermodynamic variables’, such as entropy. Unfortunately, the general definition of mechanical variables in the previous formulation [1, 2] breaks down when $||A|| = \infty$. Therefore, we here define them more physically as follows [12]. Let $A$ be a low-degree polynomial (i.e., its degree is $\Theta(1)$) of local observables. [For the order symbols, see, e.g., Ref. [4].] We make it dimensionless. For example, we denote by $\hat{H}$ the original Hamiltonian divided by an appropriate energy (such as the transfer energy). We call $A$ a mechanical variable if there exist a function $K(\beta, \mu)$ and a constant $m$, both being positive and independent
of $\hat{A}$ and $V$, such that
\[
\langle \hat{A}^2 \rangle^{\text{ens}}_{\beta \mu V} \leq K(\beta, \mu)V^{2m} \quad \text{for all } \beta, \mu, V.
\] (1)

This means that in an equilibrium state $\hat{A}$ should have finite expectation value and fluctuation even if $||\hat{A}|| = \infty$. For example, $n$-point correlation functions with $n \leq \Theta(m \ln V)$ (such as the spin-spin correlation function), and their sum (such as $\hat{H}$), are mechanical variables.

**gTPQ state** – We consider many particles confined in a box of arbitrary spatial dimensions. We assume that the grand canonical Gibbs state $\hat{\rho}^{\text{ens}}_{\beta \mu V}$ gives the correct results, which are consistent with thermodynamics [13]. This implies, for example, that specific heat is positive.

Let $\{|\nu\rangle\}_\nu$ be an arbitrary orthonormal basis of $\mathcal{H}$. Many equations (such as the main result Eq. (7) of Ref. [2]) of the previous formulation [1, 2] become ill-defined and/or meaningless when $\dim \mathcal{H} = \infty$. To overcome this difficulty, we first cut off ‘far-from equilibrium parts’ of $|\nu\rangle$ as
\[
|\nu; \beta, \mu, V\rangle \equiv \exp[-\beta(\hat{H} - \mu \hat{N})/2]|\nu\rangle,
\] (2)
where $\hat{N}$ is the number operator. We then superpose $|\nu; \beta, \mu, V\rangle$ as
\[
|\beta \mu V\rangle \equiv \sum_\nu z_\nu|\nu; \beta, \mu, V\rangle.
\] (3)

Here, $z_\nu \equiv (x_\nu + y_\nu)/\sqrt{2}$, where $x_1, x_2, \ldots$ and $y_1, y_2, \ldots$ are real random variables, each obeying the unit normal distribution. We first show that this vector is well defined, i.e., its norm is finite for finite $V$ even when $\dim \mathcal{H} = \infty$, with probability that approaches one with increasing $V$. By contrast, the norm of another random vector $\sum_\nu z_\nu|\nu\rangle$ diverges with $\dim \mathcal{H}$.

To show this, we invoke a Markov-type inequality: Let $x$ be a real random variable and $y$ a real number, then for arbitrary $\epsilon > 0$,
\[
P(|x - y| \geq \epsilon) \leq \frac{(x - y)^2}{\epsilon^2},
\] (4)
where the overbar denotes the random average. Taking $x = \langle \beta \mu V|\beta \mu V\rangle/\Xi$ and $y = 1$, where $\Xi(\beta, \mu, V)$ is the grand-partition function, we evaluate $B^2_V \equiv (\langle \beta \mu V|\beta \mu V\rangle/\Xi - 1)^2$ as
\[
B^2_V \leq 1/\exp[2V\beta\{j(T/2; \mu; V) - j(T; \mu; V)\}].
\] (5)

Here, $j(T; \mu; V) \equiv -(T/V)\ln \Xi(\beta, \mu, V)$ is a thermodynamic function, which approaches the $V$-independent one, $j(T, \mu)$, as $V \to \infty$, i.e., $j(T, \mu; V) = j(T, \mu) + o(1)$. At finite $T$, since the entropy density $s = -\partial j/\partial T = \Theta(1)$, we have
\[
2V\beta\{j(T/2; \mu; V) - j(T; \mu; V)\} \approx Vs(T, \mu) = \Theta(V).
\] (6)

Therefore, $B^2_V \leq 1/e^{V s(T, \mu)} = 1/e^{\Theta(V)}$. Inserting this result into inequality [2], we find that $\langle \beta \mu V|\beta \mu V\rangle \overset{P}{\to} \Xi(\beta, \mu, V)$, where $\overset{P}{\to}$ denotes convergence in probability. Since $\Xi$ is finite for finite $V$, $|\beta \mu V|$ is well-defined. This argument also shows that a single realization of $|\beta \mu V\rangle$ gives $j$ by
\[
- V\beta j(T, \mu; V) = \ln|\beta \mu V|\beta \mu V|,
\] (7)
with exponentially small probability of error. All genuine thermodynamic variables, such as entropy, can be calculated from $j$.

We then show that $|\beta \mu V\rangle$ is a gTPQ state, i.e.,
\[
\langle \hat{A}\rangle^{\text{TPQ}}_{\beta \mu V} \overset{P}{\to} \langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V}
\] uniformly for every mechanical variable $\hat{A}$ as $V \to \infty$, where $\langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V} = \langle \hat{A}\rangle^{\text{TPQ}}_{\beta \mu V}/|\beta \mu V|\beta \mu V|$. To see this, we take $x = \langle \hat{A}\rangle^{\text{TPQ}}_{\beta \mu V}$ and $y = \langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V}$ in inequality [2], and evaluate $D_V(A)^2 \equiv (\langle \hat{A}\rangle^{\text{TPQ}}_{\beta \mu V} - \langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V})^2$. Dropping smaller-order terms, we find
\[
D_V(A)^2 \leq \frac{(\langle \Delta \hat{A}\rangle^{\text{ens}}_{\beta \mu V})^2 + (\langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V} - \langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V})^2}{\exp[2V\beta\{j(T/2; \mu; V) - j(T; \mu; V)\}]},
\] (8)
where $(\langle \Delta \hat{A}\rangle^{\text{ens}}_{\beta \mu V})^2 = (\langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V})^2 - \langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V}^2$, and so on. The denominator of the r.h.s is $e^\Theta(V)$ from Eq. [6], whereas the numerator $\leq \Theta(V^2)$ from [1]. Hence, $D_V(A)^2 \leq V^2 e^{\Theta(V)}$, which vanishes exponentially fast with increasing $V$, for every mechanical variable $\hat{A}$. Therefore, $\langle \hat{A}\rangle^{\text{TPQ}}_{\beta \mu V} \overset{P}{\to} \langle \hat{A}\rangle^{\text{ens}}_{\beta \mu V}$ uniformly, which shows that $|\beta \mu V\rangle$ is a gTPQ state. A single realization of the gTPQ state gives equilibrium values of mechanical variables, with exponentially small probability of error, by $\langle \hat{A}\rangle^{\text{TPQ}}_{\beta \mu V}$.

Note that one can use any convenient basis as $\{|\nu\rangle\}_\nu$, because the above construction of $|\beta \mu V\rangle$ is independent of the choice of the basis. Moreover, using $j$ obtained from formula [7], one can estimate the upper bounds of errors from formulas [5] and [8], without resorting to results of other methods. This self-validating property is particularly useful in practical applications.

Similarly to the above construction of the gTPQ state, we can also generalize the cTPQ state proposed in Ref. [2] so as to be applicable to systems with $\dim \mathcal{H} = \infty$.

**Practical computational method** – The TPQ formulation sheds new light on quantum statistical mechanics because it is much different from the ensemble formulation [11]. For example, the von Neumann entropy, which coincides with the thermodynamic entropy in the ensemble formulation, vanishes for TPQ states. Because of this great difference, the TPQ formulation will also be useful for practical computations. To make this visible, we have developed practical formulas that are particularly useful for numerical computations. They are presented in Ref. [14]. Using them, one can obtain $|\beta \mu V\rangle$ simply by multiplying $[\text{constant} - (\hat{H} - \mu \hat{N})]$ with a random vector repeatedly $\Theta(N)$ times. This is a powerful numerical method, as evidenced below.
Application to the Hubbard model – We now apply the present formulation to strongly-interacting electrons. We take the Hubbard model $H = -\sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (\hat{c}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}'}^\sigma + h.c. + U \sum_{\mathbf{r}} (\hat{n}_{\mathbf{r} \uparrow} - 1/2)(\hat{n}_{\mathbf{r} \downarrow} - 1/2)$ with the periodic boundary conditions, where $\langle \mathbf{r}, \mathbf{r}' \rangle$ denotes a nearest pair of sites. We consider a 1$d$ chain and a 2$d$ triangular lattice. The number of sites $V$ is taken as $V = 14, 15$ because of the size of the memory of our computers. Although this is larger than $V$ of the numerical diagonalization (ND) ever performed (of the full spectrum to compute finite-temperature properties), the factor of Eq. (6), which appears in the r.h.s. of (5) and (8), is not large enough. In such a case, one can reduce errors by averaging the denominators and numerators, separately, of these formulas over many realizations of the gTPQ states. Averaging over $M$ realizations reduces the error by the factor of $1/\sqrt{M}$. [By contrast, averaging was not necessary for the spin system of Ref. [2] because $V (= 27, 30)$ was large enough.] We here take $10 \leq M \leq 26$.

We first study the 1$d$ chain of length $L (= V)$ as a benchmark, because some of physical quantities were exactly obtained for $L = \infty$ [13]. Since the results for $U < 0$ can be obtained from those for $U > 0$ (see, e.g., Refs. [14, 17]), we can assume $U > 0$ without loss of generality. We here take two values; $U = 1$, where the wave-particle duality plays essential roles, and $U = 8$, where the particle nature is stronger. Regarding $\mu$, it can be controlled in experiments by an external voltage [15, 21], in which $\mu$ is the electro-chemical potential. Hence, we take several values; $\mu = 0$ (half-filled), 0.5, 2, 3. $T$ is taken as $0.1 \leq T \leq 3$ (Figs. 1 and 2) and $0.03 \leq T \leq 3$ ($L = 14$ by the gTPQ state in Fig. 3). To the authors’ knowledge, no other numerical methods have ever succeeded in analyzing the Hubbard chain over such wide ranges of $T, \mu, U$ (see, e.g., Ref. [21]). One can go down to even lower $T$ by increasing the computational parameters $k_{\text{term}}$ (defined in Ref. [14]) and $M$.

The particle density $n = N/L$, obtained using the gTPQ states with $L = 15$, is plotted in Fig. 1 [We take $\mu \neq 0$ because $\mu = 0$ gives the trivial result $n = 1$.] The results agree well with the exact results for the infinite system $L \to \infty$ (broken lines) [13]. We also calculate the specific heat at constant $\mu$, defined by $c \equiv (T/L)(\partial S/\partial T)_{\mu, L}$. Generally, $c$ is much harder to compute than $n$ because $c$ is a higher (second) derivative of $j$. As shown in Fig. 2, the results of the gTPQ states with $L = 15$ agree fairly well with the exact results for $L \to \infty$ (broken lines) [13]. Small deviations are due to finite-size effects, as will be discussed later.

Furthermore, we calculate correlation functions, for which exact solutions are unknown. We calculate the charge and the staggered spin correlation functions $\phi_+$ and $\phi_-$, respectively, which are defined by

$$\phi_\pm (i) \equiv \frac{\langle \pm 1 \rangle}{L} \sum_j \langle (\hat{n}_{j \uparrow} \pm \hat{n}_{j \downarrow})(\hat{n}_{j+i \uparrow} \pm \hat{n}_{j+i \downarrow}) \rangle_{\beta \mu L}. \quad (9)$$

As shown in Fig. 3, $\phi_+$ has a dip at $i = 1$, whereas $\phi_-$ decreases monotonically with increasing $i$. These behaviors are manifestations of the wave-particle duality. $\phi_-$ was previously computed numerically in Ref. [21], where $T$ was limited to $T \leq 0.2$ and $\phi_+$ was not computed. Our results agree well with theirs.

We then study the 2$d$ triangular lattice, for which exact results are unknown. We analyze a weakly doped case ($0 < \mu \ll \text{band width}$), which will be most interesting experimentally, over a wide range of $T$. Such a case is hard to analyze with most numerical methods because of the sign problem and so on. We first solve a small system with $V = 8$, for which ND of the full spectrum is possible. In Fig. 4, the results for the specific heat $c$, obtained with ND and the gTPQ states, are plotted as a function of $T$. The agreement is very good. We then solve a larger system with $V = 15$, for which ND of the full spectrum is impossible. The result obtained with the

![FIG. 1. $n$ versus $T$, obtained by the gTPQ states with $L = 15$, for $(U, \mu, M) = (8, 2, 18), (8, 3, 20), (1, 0.5, 18)$, and $(1, 2, 22)$. Error bars show estimated errors, which can be made smaller by increasing $M$. Exact results for $L = \infty$ are also plotted.](image1)

![FIG. 2. $c$ versus $T$, obtained by the gTPQ states with $L = 15$, for $(U, \mu, M) = (8, 0.1, 14), (8, 3, 20), (1, 0.12)$, and $(1, 2, 22)$. Error bars show estimated errors, which can be made smaller by increasing $M$. Exact results for $L = \infty$ are also plotted.](image2)
gTPQ states is plotted in Fig. 4. Since we have rigorously proved that the gTPQ states give correct results (for each finite $V$) with high probability, our result is reliable within the error bars, which can be made arbitrarily small by increasing $M$ (the number of realizations). That is, we have successfully obtained reliable results for $V = 15$ over a wide range of $T$.

Superiority of the gTPQ state – We have rigorously proved that the results of a TPQ state of size $V$ agree with those of the corresponding Gibbs state of the same size $V$, within exponentially small error. However, generally, these results for a finite-size system deviate from those for an infinite system. Typically, this finite-size effect is inversely proportional to a power of $V$, and hence is not so small in general. Then a question arises: Which TPQ state has a smaller finite-size effect, the gTPQ state or the cTPQ state?

To answer this question, we compute $c$ of the 1d chain for $L = 8$ and 14, using both TPQ states. We take $\mu = 0$ (half-filled), for which $n$ is independent of $T$ ($n = 1$) and hence $c$ (at constant $\mu$) = $c$ (at constant $N$) for $L = \infty$. The results are plotted in Fig. 4. We find that the finite-size effect is much smaller in the gTPQ states than in the cTPQ states. Even for $L = 8$, the result of the gTPQ state is surprisingly close to the exact result for $L = \infty$. By contrast, the cTPQ states have very large finite-size effects even for $L = 14$. That is, the gTPQ state simulates a finite subsystem in an infinite system much better than the cTPQ state. This seems reasonable because the gTPQ state contains information about all values of $N$ whereas the cTPQ state contains information only about a specific value of $N$. Moreover, the gTPQ state also has another advantage that one can study an arbitrary value of the filling factor $\phi$.

These conclusions also apply to comparison between the canonical and grand-canonical Gibbs states in the ensemble formulation, because their results are identical to those of the cTPQ and gTPQ states, respectively (with exponentially small errors). To the authors’ knowledge, systematic studies on such comparison were not reported previously because $V$ of ND of the full spectra is severely upper bounded.

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