Canonical Thermal Pure Quantum State: Supplementary Material

Sho Sugiura and Akira Shimizu

Department of Basic Science, University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan

28 May 2013

Appendix A: Derivation of Formulas (3) - (6)

1. Random average and Variance

We calculate an average and variance of x/y, where $x = x_0 + \delta x$ and $y = y_0 + \delta y$ are random variables, x_0 and y_0 are their mean, and δx and δy are the random variables with $\overline{\delta x} = \overline{\delta y}$=0. First, we expand x/y as follows.

$$\frac{x_0 + \delta x}{y_0 + \delta y} = (x_0 + \delta x)\frac{1}{y_0}\left(1 - \frac{\delta y}{y_0} + \frac{\delta y^2}{y_0^2} - \cdots\right) \tag{A1}$$

$$= \frac{x_0}{y_0} + \frac{\delta x}{y_0} - \frac{x_0 \delta y}{y_0^2} - \frac{\delta x \delta y}{y_0^2} + \frac{x_0 \delta y^2}{y_0^3} + O(\delta^3) \tag{A2}$$

Then, the average of x/y is

$$\overline{\left(\frac{x_0 + \delta x}{y_0 + \delta y}\right)} = \frac{x_0}{y_0} - \frac{\overline{\delta x \delta y}}{y_0^2} + \frac{x_0 \overline{\delta y^2}}{y_0^3} + O(\overline{\delta^3}) \tag{A3}$$

and the variance is

$$\overline{\left(\frac{x_0 + \delta x}{y_0 + \delta y} - \overline{\left(\frac{x_0 + \delta x}{y_0 + \delta y}\right)}\right)^2} = \overline{\left(\frac{\delta x}{y_0} - \frac{x_0 \delta y}{y_0^2}\right)^2} + O(\overline{\delta^3}) \tag{A4}$$

$$= \frac{\overline{\delta x^2}}{y_0^2} - 2\frac{x_0 \overline{\delta x \delta y}}{y_0^3} + \frac{x_0^2 \overline{\delta y^2}}{y_0^4} + O(\overline{\delta^3}) \tag{A5}$$

Therefore, we need 3 terms, $\overline{\delta x^2}$, $\overline{\delta x \delta y}$, and $\overline{\delta y^2}$, to calculate an average and variance of the form x/y up to the order of $O(\overline{\delta^2})$. In the following subsections, we calculate these terms.

Before starting the respective calculation, we derive a frequently used formula. We calculate

$$\overline{\left(\langle\psi_0|\hat{B}|\psi_0\rangle - \overline{\langle\psi_0|\hat{B}|\psi_0\rangle}\right)\left(\langle\psi_0|\hat{C}|\psi_0\rangle - \overline{\langle\psi_0|\hat{C}|\psi_0\rangle}\right)} \tag{A6}$$

where $\hat{B}$ and $\hat{C}$ are arbitrary operators. Using the formula of random matrix theory in N. Ullah, Nucl. Phys. **58**, 65

(1964), we get

$$\begin{aligned}
&\overline{\left(\langle\psi_0|\hat{B}|\psi_0\rangle - \overline{\langle\psi_0|\hat{B}|\psi_0\rangle}\right)\left(\langle\psi_0|\hat{C}|\psi_0\rangle - \overline{\langle\psi_0|\hat{C}|\psi_0\rangle}\right)} \\
&= \sum_{n,m,n',m'} \overline{c_n^* c_m c_{n'}^* c_{m'}} \langle n|\hat{B}|m\rangle\langle n'|\hat{C}|m'\rangle \\
&\quad - \sum_{n,m} \overline{c_n^* c_m}\langle n|\hat{B}|m\rangle \sum_{n',m'} \overline{c_{n'}^* c_{m'}}\langle n'|\hat{C}|m'\rangle \qquad \text{(A7)} \\
&= \sum_n \overline{|c_n|^4}\langle n|\hat{B}|n\rangle\langle n|\hat{C}|n\rangle + \sum_{n\neq n'} \overline{|c_n|^2|c_{n'}|^2}\langle n|\hat{B}|n\rangle\langle n'|\hat{C}|n'\rangle \\
&\quad + \sum_{n\neq m} \overline{|c_n|^2|c_m|^2}\langle n|\hat{B}|m\rangle\langle m|\hat{C}|n\rangle - \sum_n \overline{|c_n|^2}\langle n|\hat{B}|n\rangle \sum_{n'} \overline{|c_{n'}|^2}\langle n'|\hat{C}|n'\rangle \\
&= \frac{2}{D(D+1)}\sum_n \langle n|\hat{B}|n\rangle\langle n|\hat{C}|n\rangle + \frac{1}{D(D+1)}\sum_{n\neq m}\langle n|\hat{B}|n\rangle\langle m|\hat{C}|m\rangle \\
&\quad + \frac{1}{D(D+1)}\sum_{n\neq m}\langle n|\hat{B}|m\rangle\langle m|\hat{C}|n\rangle - \frac{1}{D^2}\sum_{n,m}\langle n|\hat{B}|n\rangle\langle m|\hat{C}|m\rangle \qquad \text{(A8)} \\
&= \frac{1}{D(D+1)}\sum_{n,m}\langle n|\hat{B}|n\rangle\langle m|\hat{C}|m\rangle + \frac{1}{D(D+1)}\sum_{n,m}\langle n|\hat{B}|m\rangle\langle m|\hat{C}|n\rangle \\
&\quad - \frac{1}{D^2}\sum_{n,m}\langle n|\hat{B}|n\rangle\langle m|\hat{C}|m\rangle \qquad \text{(A9)} \\
&= \frac{1}{D(D+1)}\sum_{n,m}\langle n|\hat{B}|m\rangle\langle m|\hat{C}|n\rangle - \frac{1}{D^2(D+1)}\sum_{n,m}\langle n|\hat{B}|n\rangle\langle m|\hat{C}|m\rangle \qquad \text{(A10)}
\end{aligned}$$

Here, we take $|n\rangle$ as a energy eigenstate such that $\hat{h}|n\rangle = e_n|n\rangle$.

2. Normalization Constant (Partition Function)

Now, we prove that canonical TPQ states $|\beta, N\rangle \equiv \exp(-N\beta\hat{h}/2)|\psi_0\rangle$ give the correct equilibrium values from the normalization constant and the expectation values. Firstly, we see $\langle\beta, N|\beta, N\rangle$, which works like a partition function. Its average behaves as

$$\overline{\langle\beta, N|\beta, N\rangle} = \frac{1}{D}\sum_n \exp(-N\beta e_n) \qquad \text{(A11)}$$

$$= \frac{1}{D}Z(\beta, N) \qquad \text{(A12)}$$

where we denote $Z(\beta, N) \equiv \sum_n \exp[-N\beta e_n]$. Then, we see its variance.

$$\overline{(\langle\beta, N|\beta, N\rangle - \overline{\langle\beta, N|\beta, N\rangle})^2} \qquad \text{(A13)}$$

This is the case of $\hat{B} = \hat{C} = \exp[-N\beta\hat{h}]$ in the expression (A6). Thus, we get

$$\begin{aligned}
&\overline{(\langle\beta, N|\beta, N\rangle - \overline{\langle\beta, N|\beta, N\rangle})^2} \\
&= \frac{1}{D(D+1)}\sum_n \langle n|\exp[-2N\beta\hat{h}]|n\rangle - \frac{1}{D^2(D+1)}\left(\sum_n \langle n|\exp[-N\beta\hat{h}]|n\rangle\right)^2 \qquad \text{(A14)} \\
&= \frac{1}{D(D+1)}\sum_n \exp[-2N\beta e_n] - \frac{1}{D^2(D+1)}\left(\sum_n \exp[-N\beta e_n]\rangle\right)^2 \qquad \text{(A15)} \\
&= \frac{1}{D(D+1)}Z(2\beta, N) - \frac{1}{D^2(D+1)}Z(\beta, N)^2 \qquad \text{(A16)}
\end{aligned}$$

In order to see the variance of $\langle \beta, N|\beta, N\rangle$ is negligible comparing to the average, we divide the variance by the squared average.

$$\frac{\frac{1}{D(D+1)}Z(2\beta,N)-\frac{1}{D^2(D+1)}Z(\beta,N)^2}{\left(\frac{1}{D}Z(\beta,N)\right)^2} \tag{A17}$$

$$\leq \frac{D}{(D+1)}\frac{Z(2\beta,N)}{Z(\beta,N)^2} \tag{A18}$$

$$= \frac{D}{(D+1)}\frac{1}{\exp(2N\beta(f(1/2\beta;N)-f(1/\beta;N)))} \tag{A19}$$

where $f(T;N)$ is the free energy density and $f(0;N)-f(1/\beta;N)>0$ is $O(1)$. Hence, we finally get

$$\mathrm{Prob}\left(\left|\langle \beta, N|\beta, N\rangle/\overline{\langle \beta, N|\beta, N\rangle}-1\right|\geq\epsilon\right)$$
$$\leq \frac{1}{\epsilon^2}\frac{D}{(D+1)}\frac{1}{\exp[2N\beta(f(1/2\beta;N)-f(1/\beta;N))]} \tag{A20}$$

Here we derive Eq.(6). ¿From a canonical TPQ state, we can get the partition function with negligible error.

3. Mechanical Variables

Then, we consider the average and the variance of $\langle \beta, N|\hat{A}|\beta, N\rangle/\langle \beta, N|\beta, N\rangle$. ¿From Eq. (A3) and Eq. (A5), we need to calculate these two,

$$\overline{\left(\langle \beta, N|\hat{A}|\beta, N\rangle-\overline{\langle \beta, N|\hat{A}|\beta, N\rangle}\right)^2} \tag{A21}$$

$$\overline{\left(\langle \beta, N|\hat{A}|\beta, N\rangle-\overline{\langle \beta, N|\hat{A}|\beta, N\rangle}\right)\left(\langle \beta, N|\beta, N\rangle-\overline{\langle \beta, N|\beta, N\rangle}\right)} \tag{A22}$$

First, we calculate the term (A21). Using Eq. (A10) with $\hat{B}=\hat{C}=\exp[-\frac{1}{2}N\beta\hat{h}]\hat{A}\exp[-\frac{1}{2}N\beta\hat{h}]$, we get

$$\overline{\left(\langle \beta, N|\hat{A}|\beta, N\rangle-\overline{\langle \beta, N|\hat{A}|\beta, N\rangle}\right)^2}$$
$$=\frac{1}{D(D+1)}\sum_n\langle n|\exp[-\frac{1}{2}N\beta\hat{h}]\hat{A}\exp[-N\beta\hat{h}]\hat{A}\exp[-\frac{1}{2}N\beta\hat{h}]|n\rangle$$
$$-\frac{1}{D^2(D+1)}\left(\sum_n\langle n|\exp[-\frac{1}{2}N\beta\hat{h}]\hat{A}\exp[-\frac{1}{2}N\beta\hat{h}]|n\rangle\right)^2 \tag{A23}$$
$$=\frac{1}{D(D+1)}\sum_n\exp(-N\beta e_n)\langle n|\hat{A}\exp(-N\beta\hat{h})\hat{A}|n\rangle$$
$$-\frac{1}{D^2(D+1)}\left(\langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N}Z(\beta,N)\right)^2 \tag{A24}$$

where we denote $\langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N}\equiv\sum_n\exp(-N\beta e_n)\langle n|\hat{A}|n\rangle$.

Then, we calculate the term (A22). Using Eq. (A10) with $\hat{B}=\exp[-\frac{1}{2}N\beta\hat{h}]\hat{A}\exp[-\frac{1}{2}N\beta\hat{h}]$ and $\hat{C}=\exp[-N\beta\hat{h}]$, we get

$$\overline{\left(\langle\beta,N|\hat{A}|\beta,N\rangle-\overline{\langle\beta,N|\hat{A}|\beta,N\rangle}\right)\left(\langle\beta,N|\beta,N\rangle-\overline{\langle\beta,N|\beta,N\rangle}\right)}$$

$$=\frac{1}{D(D+1)}\sum_n\langle n|\exp[-\frac{1}{2}N\beta\hat{h}]\hat{A}\exp[-\frac{3}{2}N\beta\hat{h}]|n\rangle$$
$$-\frac{1}{D^2(D+1)}\sum_n\langle n|\exp[-\frac{1}{2}N\beta\hat{h}]\hat{A}\exp[-\frac{1}{2}N\beta\hat{h}]|n\rangle\sum_n\langle n|\exp[-N\beta\hat{h}]|n\rangle \tag{A25}$$

$$=\frac{1}{D(D+1)}\sum_n\exp(-2N\beta e_n)\langle n|\hat{A}|n\rangle$$
$$-\frac{1}{D^2(D+1)}\sum_n\exp(-N\beta e_n)\langle n|\hat{A}|n\rangle\sum_n\exp(-N\beta e_n) \tag{A26}$$

$$=\frac{1}{D(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{2\beta,N}Z(2\beta,N)-\frac{1}{D^2(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}Z(\beta,N)^2 \tag{A27}$$

Here, we are ready to evaluate the average and the variance of $\langle\beta,N|\hat{A}|\beta,N\rangle/\langle\beta,N|\beta,N\rangle$.

a. mean

Using Eq. (A3), (A16), and (A27), we get the average

$$\overline{\langle\hat{A}\rangle^{\text{TPQ}}_{\beta,N}}-\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}$$

$$=-\frac{1}{D(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{2\beta,N}Z(2\beta,N)/\overline{\langle\beta,N|\beta,N\rangle}^2+\frac{1}{D^2(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}Z(\beta,N)^2/\overline{\langle\beta,N|\beta,N\rangle}^2$$
$$+\frac{1}{D(D+1)}Z(2\beta,N)\overline{\langle\beta,N|\hat{A}|\beta,N\rangle}/\overline{\langle\beta,N|\beta,N\rangle}^3-\frac{1}{D^2(D+1)}Z(\beta,N)^2\overline{\langle\beta,N|\hat{A}|\beta,N\rangle}/\overline{\langle\beta,N|\beta,N\rangle}^3 \tag{A28}$$

$$=-\frac{1}{D(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{2\beta,N}Z(2\beta,N)/\left(\frac{1}{D}Z(\beta,N)\right)^2+\frac{1}{D^2(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}Z(\beta,N)^2/\left(\frac{1}{D}Z(\beta,N)\right)^2$$
$$+\frac{1}{D(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}Z(2\beta,N)/\left(\frac{1}{D}Z(\beta,N)\right)^2-\frac{1}{D^2(D+1)}\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}Z(\beta,N)^2/\left(\frac{1}{D}Z(\beta,N)\right)^2 \tag{A29}$$

Here, we negligible $O(\delta^3)$ terms in Eq. (A3). Then, we get

$$\overline{\langle\hat{A}\rangle^{\text{TPQ}}_{\beta,N}}-\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}=-\frac{1}{D(D+1)}\left(\langle\hat{A}\rangle^{\text{ens}}_{2\beta,N}-\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}\right)Z(2\beta,N)/\left(\frac{1}{D}Z(\beta,N)\right)^2 \tag{A30}$$

$$=\frac{-D^2}{D(D+1)}Z(2\beta,N)\left(\langle\hat{A}\rangle^{\text{ens}}_{2\beta,N}-\langle\hat{A}\rangle^{\text{ens}}_{\beta,N}\right)/Z(\beta,N)^2 \tag{A31}$$

$$=\frac{D}{D+1}\frac{\langle\hat{A}\rangle_{\text{can}}(\beta)-\langle\hat{A}\rangle_{\text{can}}(2\beta)}{\exp[2N\beta(f(1/2\beta;N)-f(1/\beta;N))]} \tag{A32}$$

b. variance

Using Eq. (A5), (A16), (A24), and (A27), we get the variance

$$
\begin{aligned}
&\overline{\left(\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}-\overline{\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}}\right)^2}\\
&=\frac{1}{D(D+1)}\sum_n \exp(-N\beta e_n)\langle n|\hat{A}\exp(-N\beta\hat{h})\hat{A}|n\rangle/\overline{\langle\beta,N|\beta,N\rangle}^2\\
&-\frac{1}{D^2(D+1)}\left(\langle\hat{A}\rangle^{\rm ens}_{\beta,N}Z(\beta,N)\right)^2/\overline{\langle\beta,N|\beta,N\rangle}^2\\
&-2\frac{1}{D(D+1)}\langle\hat{A}\rangle^{\rm ens}_{\beta,N}\langle\hat{A}\rangle^{\rm ens}_{2\beta,N}Z(2\beta,N)/\overline{\langle\beta,N|\beta,N\rangle}^2+2\frac{1}{D^2(D+1)}\left(\langle\hat{A}\rangle^{\rm ens}_{\beta,N}Z(\beta,N)\right)^2/\overline{\langle\beta,N|\beta,N\rangle}^2\\
&+\frac{1}{D(D+1)}(\langle\hat{A}\rangle^{\rm ens}_{\beta,N})^2Z(2\beta,N)/\overline{\langle\beta,N|\beta,N\rangle}^2-\frac{1}{D^2(D+1)}\left(\langle\hat{A}\rangle^{\rm ens}_{\beta,N}Z(\beta,N)\right)^2/\overline{\langle\beta,N|\beta,N\rangle}^2 \qquad \text{(A33)}\\
&=\frac{1}{D(D+1)(\frac{1}{D}Z(\beta,N))^2}\left(\left\{\sum_n \exp(-N\beta e_n)\langle n|\hat{A}\exp(-N\beta\hat{h})\hat{A}|n\rangle\right\}\right.\\
&\qquad\left.-2\langle\hat{A}\rangle^{\rm ens}_{\beta,N}\langle\hat{A}\rangle^{\rm ens}_{2\beta,N}Z(2\beta,N)+(\langle\hat{A}\rangle^{\rm ens}_{\beta,N})^2Z(2\beta,N)\right) \qquad \text{(A34)}
\end{aligned}
$$

If we number e_n s.t. $e_n \le e_{n'}$ for $n<n'$, we have

$$
\begin{aligned}
\{\ \}\text{ in Eq. (A34)} &= \sum_{m,n}|\langle n|\hat{A}|m\rangle|^2 e^{-N\beta(e_n+e_m)} &\text{(A35)}\\
&\le \sum_{m,n}|\langle n|\hat{A}|m\rangle|^2\frac{e^{-2N\beta e_m}+e^{-2N\beta e_n}}{2} &\text{(A36)}\\
&=\frac{1}{2}\sum_m\langle m|\hat{A}^2|m\rangle e^{-2N\beta e_m}+\frac{1}{2}\sum_n\langle n|\hat{A}^2|n\rangle e^{-2N\beta e_n}\\
&=\langle\hat{A}^2\rangle^{\rm ens}_{2\beta,N}Z(2\beta,N). &\text{(A37)}
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\overline{\left(\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}-\overline{\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}}\right)^2} &\le \frac{D}{D+1}\cdot\frac{Z(2\beta,N)}{Z(\beta,N)^2}\left(\langle\hat{A}^2\rangle^{\rm ens}_{2\beta,N}-2\langle\hat{A}\rangle^{\rm ens}_{\beta,N}\langle\hat{A}\rangle^{\rm ens}_{2\beta,N}+(\langle\hat{A}\rangle^{\rm ens}_{\beta,N})^2\right) &\text{(A38)}\\
&\le \frac{D}{D+1}\cdot\frac{Z(2\beta,N)}{Z(\beta,N)^2}\\
&\quad\times\left(\langle(\hat{A}-\langle\hat{A}\rangle^{\rm ens}_{2\beta,N})^2\rangle^{\rm ens}_{2\beta,N}+[\langle\hat{A}\rangle^{\rm ens}_{\beta,N}-\langle\hat{A}\rangle^{\rm ens}_{2\beta,N}]^2\right) &\text{(A39)}\\
&=\frac{D}{D+1}\frac{\langle(\Delta\hat{A})^2\rangle^{\rm ens}_{2\beta,N}+[\langle\hat{A}\rangle^{\rm ens}_{\beta,N}-\langle\hat{A}\rangle^{\rm ens}_{2\beta,N}]^2}{\exp[2N\beta(f(1/2\beta;N)-f(1/\beta;N))]}, &\text{(A40)}
\end{aligned}
$$

where

$$\langle(\Delta\hat{A})^2\rangle^{\rm ens}_{2\beta,N}\equiv\langle(\hat{A}-\langle\hat{A}\rangle^{\rm ens}_{2\beta,N})^2\rangle^{\rm ens}_{2\beta,N}. \qquad \text{(A41)}$$

c. Derivation of inequality. (3)

Using Eq. (A32) and (A40), we derive inequality (3).

$$
\begin{aligned}
D_N(A) &= \overline{\left(\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}-\overline{\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}}\right)^2}+\left|\overline{\langle\hat{A}\rangle^{\rm TPQ}_{\beta,N}}-\langle\hat{A}\rangle^{\rm ens}_{\beta,N}\right|^2 &\text{(A42)}\\
&\le \frac{D}{D+1}\frac{\langle(\Delta\hat{A})^2\rangle^{\rm ens}_{2\beta,N}+[\langle\hat{A}\rangle^{\rm ens}_{\beta,N}-\langle\hat{A}\rangle^{\rm ens}_{2\beta,N}]^2}{\exp[2N\beta(f(1/2\beta;N)-f(1/\beta;N))]} &\text{(A43)}
\end{aligned}
$$

At the last line, we drop smaller-order term comes from $\left|\overline{\langle \hat{A} \rangle^{\mathrm{TPQ}}_{\beta,N}} - \langle \hat{A} \rangle^{\mathrm{ens}}_{\beta,N}\right|^2$.

Note that the RHS vanishes when

$$\langle (\Delta \hat{A})^2 \rangle^{\mathrm{ens}}_{2\beta,N} = 0 \;\text{ and }\; \langle \hat{A} \rangle^{\mathrm{ens}}_{\beta,N} = \langle \hat{A} \rangle^{\mathrm{ens}}_{2\beta,N}. \tag{A44}$$

Appendix B: Properties of expansion (10)

In this section, we will use the same notation as in Ref. [6], e.g.,

$$\kappa \equiv k/N, \tag{B1}$$

$$\xi_\kappa(u; N) \equiv s(u; N) + 2\kappa \ln(l - u). \tag{B2}$$

By taking the energy eigenstates $\{|n\rangle\}_n$ ($\hat{h}|n\rangle = e_n|n\rangle$) as the arbitrary basis $\{|i\rangle\}_i$ used in the construction of $|\psi_0\rangle$, we have

$$Q_k = \sum_n |c_n|^2 (l - e_n)^{2k} \sim \frac{1}{\lambda^N} \sum_n (l - e_n)^{2k} \tag{B3}$$

from the law of large numbers. We can investigate the behavior of Q_k, in a way similar to Ref. [6], as follows.

Dropping exponentially small terms, we have

$$Q_k = \frac{1}{\lambda^N} \int e^{N\xi_\kappa(u;N)} du \tag{B4}$$

$$\sim \frac{1}{\lambda^N} e^{N\xi_\kappa(u^*_\kappa;N)} \int \exp\left[-\frac{N}{2}|\xi''_\kappa|(u - u^*_\kappa)^2\right] du \tag{B5}$$

$$= \frac{1}{\lambda^N} \sqrt{\frac{2\pi}{N|\xi''_\kappa|}} e^{N\xi_\kappa(u^*_\kappa;N)}. \tag{B6}$$

Here, u^*_κ is defined as the solution of

$$\beta(u; N) = \frac{2\kappa}{l - u}, \tag{B7}$$

where

$$\beta(u; N) \equiv \frac{\partial}{\partial u} s(u; N). \tag{B8}$$

That is, u^*_κ satisfies

$$\beta(u^*_\kappa; N) = \frac{2\kappa}{l - u^*_\kappa}, \tag{B9}$$

It was shown in Ref. [6] that u^*_κ is close to u_κ as

$$u^*_\kappa = u_\kappa + O(1/N). \tag{B10}$$

Note that these results are valid even when a first-order phase transition takes place, as discussed in Sec. C.

Using Eq. (B6) and Starling's formula, we have

$$R_k \sim \exp\left[\frac{N}{2}\zeta_\kappa(\beta; N)\right], \tag{B11}$$

where

$$\zeta_\kappa(\beta; N) \equiv \xi_\kappa(u^*_\kappa; N) - \ln 2 + 2\kappa + 2\kappa \ln(\beta/2\kappa). \tag{B12}$$

Here, β in the rhs is not a function $\beta(u^*_\kappa; N)$ but an independent parameter of the canonical TPQ state. If κ took continuous values, ζ_κ would take maximum at κ_{**} such that

$$\beta(u^*_{\kappa_{**}}; N) = \beta. \tag{B13}$$

This can be shown by taking derivative of $\zeta_\kappa(\beta;N)$ of Eq. (B11) as

$$\frac{\partial}{\partial\kappa}\zeta_\kappa(\beta;N) = \left[\beta(u_\kappa^*;N) - \frac{2\kappa}{(l-u_\kappa^*)}\right]\frac{\partial u_\kappa^*}{\partial\kappa} + 2\ln\left[\beta \middle/ \frac{2\kappa}{(l-u_\kappa^*)}\right] \tag{B14}$$

$$= 2\ln\left[\frac{\beta}{\beta(u_\kappa^*;N)}\right]. \tag{B15}$$

As κ is increased, u_κ^* decreases and $\beta(u_\kappa^*;N)$ increases. Therefore, with increasing κ, this derivative decreases monotonically from positive values (for $\kappa < \kappa_{**}$), to zero (at $\kappa = \kappa_{**}$), and to negative values (for $\kappa > \kappa_{**}$). Hence, R_k takes maximum at $\kappa = \kappa_{**}$, if κ takes continuous values.

Although κ actually takes discrete values ($= 0, 1/N, 2/N, \cdots$), we can find a value(s) κ_* among these values such that $\left|\frac{\partial}{\partial\kappa}\zeta_\kappa(\beta;N)\right|$ is minimum. u_κ also takes discrete values, whose intervals are

$$u_{\kappa\pm1/N} - u_\kappa = O(1/N). \tag{B16}$$

Hence, from Eq. (B10),

$$u^*_{\kappa\pm1/N} - u^*_\kappa = O(1/N). \tag{B17}$$

Therefore,

$$u^*_{\kappa_*} - u^*_{\kappa_{**}} = O(1/N), \tag{B18}$$
$$\beta(u^*_{\kappa_*};N) = \beta + O(1/N). \tag{B19}$$

Since $\beta(u;N) = \Theta(1)$, there exists a constant $\Delta\kappa$ of $\Theta(1)$ such that

$$\frac{\partial}{\partial\kappa}\zeta_\kappa(\beta;N) = \begin{cases}\Theta(1) & (\kappa \le \kappa_* - \Delta\kappa),\\ -\Theta(1) & (\kappa \ge \kappa_* + \Delta\kappa)\end{cases} \tag{B20}$$

Therefore, there exists a positive constant η of $\Theta(1)$ such that

$$\zeta_{\kappa_*}(\beta;N) - \zeta_\kappa(\beta;N) \ge \eta|\kappa-\kappa_*| \quad \text{for } |\kappa-\kappa_*| \ge \Delta\kappa. \tag{B21}$$

Hence, for $\kappa - \kappa_* \ge \Delta\kappa$, we have the asymptotic inequality

$$|R_k| \le \exp\left[\frac{N}{2}\zeta_{\kappa_*}(\beta;N)\right]\exp\left[-\frac{N}{2}\eta(\kappa-\kappa_*)\right] \tag{B22}$$

$$= \exp\left[\frac{N}{2}\zeta_{\kappa_*}(\beta;N)\right]\exp\left[-\frac{\eta}{2}(k-k_*)\right], \tag{B23}$$

where $k_* \equiv N\kappa_*$. We take $k_{\max}$ arbitrarily such that

$$k_{\max} \ge k_* + N\Delta\kappa. \tag{B24}$$

Then we have

$$\left\|\sum_{k\ge k_{\max}} R_k|\psi_k\rangle\right\| \le \sum_{k\ge k_{\max}} R_k \tag{B25}$$

$$\le \exp\left[\frac{N}{2}\zeta_{\kappa_*}(\beta;N)\right]\exp\left[\frac{\eta}{2}k_*\right]\sum_{k\ge k_{\max}}\exp\left[-\frac{\eta}{2}k\right] \tag{B26}$$

$$= \exp\left[\frac{N}{2}\zeta_{\kappa_*}(\beta;N)\right]\exp\left[\frac{\eta}{2}(k_*-k_{\max})\right]\frac{1}{1-e^{-\eta/2}}, \tag{B27}$$

which vanishes as $k_{\max} \to \infty$. Since k_* is a function of β and $k_{\max} > k_*$, this means that the series converges quickly for each value of β. Therefore, if we take arbitrarily the upper bound $\beta_{\max}$ of β, then the series converges uniformly for all β such that $0 < \beta \le \beta_{\max}$.

Appendix C: Note on the first-order phase transition

Note that

$$\frac{\partial}{\partial u}\beta(u;N) \leq 0 \tag{C1}$$

holds asymptotically, where the equality holds only at a first-order phase transition. Hence,

$$\frac{\partial^2}{\partial u^2}\xi_\kappa(u;N) = \frac{\partial}{\partial u}\beta(u;N) - \frac{2\kappa}{(l-u)^2} < 0 \tag{C2}$$

holds for every finite u, even at a first-order phase transition. As a result, Eq. (B6) is valid even when a first-order phase transition takes place. (This is an advantage of our introducing l!)

That is, at a first-order phase transition $\beta(u^*_\kappa;N)$ takes the same value for multiple values of κ (and u^*_κ). For each of such κ, however, Eq. (B6) is valid. and the solution u^*_κ of Eq. (B7) is determined uniquely.

At a first-order phase transition an equilibrium state cannot be specified by (β, N) uniquely. [See Ref.[10] for complete discussions, and Ref.[18] for a hint.] To specify an equilibrium state uniquely, one must use (u, N) instead of (β, N). As a result of this fact, neither the canonical density operator (of the ensemble formulation) nor the canonical TPQ state (of our formulation) can specify an equilibrium state uniquely. One must use either the microcanonical density operator (of the ensemble formulation) nor the microcanonical TPQ state (of our formulation) to specify an equilibrium state uniquely, at a first-order phase transition.

Nevertheless, one can use the canonical density operator (of the ensemble formulation) or the canonical TPQ state (of our formulation) even at a first-order phase transition, because they give the correct free energy, from which the entropy function (the fundamental relation) can be obtained by the Legendre transformation [10]. As a result, all the formulas of our paper are valid even at a first-order phase transition.