Thermal Pure Quantum States of Many-Particle Systems: *Supplemental Material*

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Practical formulas for numerical computation using the grand-canonical thermal pure quantum (gTPQ) states are presented.

In numerical computations, one has to introduce a certain cutoff to make $\dim\mathcal{H}$ finite. Then, $\hat{g}\equiv(\hat{H}-\mu\hat{N})/V$ has the maximum eigenvalue $g_{\max}$, and we can arbitrarily take a number l such that $l\geq g_{\max}$. Using l, we define

$$|k\rangle\equiv\sum_{\nu}z_{\nu}(l-\hat{g})^{k}|\nu\rangle\quad(k=0,1,2,\ldots),\tag{1}$$

and the normalized one, $|\psi_k\rangle\equiv(1/\sqrt{Q_k})|k\rangle$, where $Q_k\equiv\langle k|k\rangle$. If $\hat{g}$ is replaced with $\hat{H}/V$, $|\psi_k\rangle$ reduces to the mTPQ state of Ref. [1]. Hence, we simply call $|k\rangle$ and $|\psi_k\rangle$ mTPQ states. We have

$$e^{V\beta l/2}|\beta\mu V\rangle=\sum_{k=0}^{\infty}\frac{(V\beta/2)^k}{k!}|k\rangle=\sum_{k=0}^{\infty}R_k|\psi_k\rangle,\tag{2}$$

where $R_k\equiv(V\beta/2)^k\sqrt{Q_k}/k!$. We can prove that this sum is uniformly convergent on any finite interval of β. We can also prove that R_k takes significant values only for k such that

$$\langle\psi_k|\hat{g}|\psi_k\rangle=\langle\hat{g}\rangle_{\beta\mu V}^{\rm TPQ}+O(1/V).\tag{3}$$

As k moves away from such values, R_k vanishes exponentially fast. This means that $|\beta\mu V\rangle$ is almost composed of $|\psi_k\rangle$'s which represent the same equilibrium state as that represented by $|\beta\mu V\rangle$. Therefore, one can terminate the sum at a finite number $k_{\rm term}$, which depends on the largest β of interest, $\beta_{\max}$. For any $\beta_{\max}=\Theta(1)$, we can show that $k_{\rm term}=\Theta(N)$. Since $|\psi_1\rangle,|\psi_2\rangle,\cdots,|\psi_{k_{\rm term}}\rangle$ can be obtained iteratively by simply multiplying $(l-\hat{g})$ with a random vector $k_{\rm term}$ times [1], one can obtain $|\beta\mu V\rangle$ by multiplying $(l-\hat{g})$ repeatedly $\Theta(N)$ times.

We can obtain more practical formulas. Let

$$\{\hat{A}\}'_{\beta\mu V}\equiv\sum_{k=0}^{\infty}\left[\frac{(V\beta)^{2k}}{(2k)!}\langle k|\hat{A}|k\rangle+\frac{(V\beta)^{2k+1}}{(2k+1)!}\langle k|\hat{A}|k+1\rangle\right].\tag{4}$$

When $[\hat{A},\hat{g}]=0$, we have

$$\{\hat{A}\}'_{\beta\mu V}=\langle\beta\mu V|\hat{A}|\beta\mu V\rangle.\tag{5}$$

For example, $\{\hat{1}\}'_{\beta\mu V}=\langle\beta\mu V|\beta\mu V\rangle$. Even when $[\hat{A},\hat{g}]\neq0$, the above equality is almost exact. To see this, we take $x=\{\hat{A}\}_{\beta\mu V}^{\rm TPQ}\equiv\{\hat{A}\}'_{\beta\mu V}/\{\hat{1}\}'_{\beta\mu V}$ and $y=\langle\hat{A}\rangle_{\beta\mu V}^{\rm ens}$ in inequality (3) of the paper, and evaluate

$$E_V(A)^2\equiv\overline{(\{\hat{A}\}_{\beta\mu V}^{\rm TPQ}-\langle\hat{A}\rangle_{\beta\mu V}^{\rm ens})^2}\tag{6}$$

as

$$E_V(A)^2\leq\frac{\langle(\Delta\hat{A})^2\rangle_{\beta\mu V}^{\rm ens}}{\exp[V\beta\{j(0,\mu;V)-j(T,\mu;V)\}]}.\tag{7}$$

This shows that

$$E_V(A)^2\leq V^{2m}/e^{\Theta(V)}\tag{8}$$

and $\{\hat{A}\}_{\beta\mu V}^{\rm TPQ}\overset{P}{\to}\langle\hat{A}\rangle_{\beta\mu V}^{\rm ens}$ exponentially fast and uniformly. With this formula one needs only to calculate $\langle k|\hat{A}|k\rangle$ and $\langle k|\hat{A}|k+1\rangle$ for all $k\leq k_{\rm term}$ to obtain the results for *all* $\beta\leq\beta_{\max}$.

When computer resources are not sufficient to treat large enough V, it may be possible that $E_V(A)^2$ is not small enough. As described in the paper, in such a case one can reduce errors by averaging over many realizations of the gTPQ states because

$$\ln\overline{\langle\beta\mu V|\beta\mu V\rangle}=-V\beta j(1/\beta,\mu;V),\tag{9}$$

$$\frac{\overline{\langle\beta\mu V|\hat{A}|\beta\mu V\rangle}}{\overline{\langle\beta\mu V|\beta\mu V\rangle}}=\frac{\overline{\{\hat{A}\}'_{\beta\mu V}}}{\overline{\{\hat{1}\}'_{\beta\mu V}}}=\langle\hat{A}\rangle_{\beta\mu V}^{\rm ens}.\tag{10}$$

Averaging over M realizations reduces the error by the factor of $1/\sqrt{M}$.

Note that averages should be taken as indicated in Eqs. (9) and (10). Otherwise, averages would not approach the correct values as shown in Supplemental Material of Ref. [2].

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[1] S. Sugiura and A. Shimizu, Phys. Rev. Lett. **108**, 240401 (2012).
[2] S. Sugiura and A. Shimizu, Phys. Rev. Lett. **111**, 010401 (2013).