Note on TPQ state

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In this note, we show how to construct the spin grand canonical thermal pure quantum (TPQ) state from the superposition of the S_z conserved TPQ states.

1. Relation between S_z conserved TPQ states and spin grand canonical TPQ state

Let $|\Phi_0\rangle$ be the random vector in the total Hilbert space and $|\phi_0^{S_z}\rangle$ be the random vector in fixed S_z Hilbert space. The relation between them is given as follows.

$$|\Phi_0\rangle = \sum_{S_z} |\phi_0^{S_z}\rangle = \sum_{S_z}\sum_{x} C_x^{S_z}|x^{S_z}\rangle, \tag{1}$$

where $|x^{S_z}\rangle$ is real-space configuration with S_z and $C_x^{S_z}$ is coefficient.

Norms of them are given as follows.

$$(d_0^{S_z})^2 = \langle\phi_0^{S_z}|\phi_0^{S_z}\rangle = \sum_{x}|C_x^{S_z}|^2 \tag{2}$$

$$(D_0)^2 = \langle\Phi_0|\Phi_0\rangle = \sum_{S_z,x}|C_x^{S_z}|^2 = \sum_{S_z}(d_0^{S_z})^2 \tag{3}$$

By using these norms, normalized vectors are are given as follows.

$$|\bar{\phi}_0^{S_z}\rangle = \frac{1}{d_0^{S_z}}|\phi_0^{S_z}\rangle \tag{4}$$

$$|\bar{\Phi}_0\rangle = \frac{1}{D_0}|\Phi_0\rangle = \sum_{S_z}\frac{d_0^{S_z}}{D_0}|\bar{\phi}_0^{S_z}\rangle \tag{5}$$

From these random vectors, we construct TPQ state by successively multiplying $(l-\hat{h})$.

$$|\phi_1^{S_z}\rangle = (l-\hat{h})|\bar{\phi}_0\rangle, \tag{6}$$

$$|\Phi_1\rangle = (l-\hat{h})|\bar{\Phi}_0\rangle = \sum_{S_z}\frac{d_0^{S_z}}{D_0}(l-\hat{h})|\bar{\phi}_0^{S_z}\rangle = \sum_{S_z}\frac{d_0^{S_z}}{D_0}|\phi_1^{S_z}\rangle \tag{7}$$

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Normalization of TPQ states are give as follows.

$$(d_1^{S_z})^2 = \langle\phi_1|\phi_1\rangle, \quad (D_1)^2 = \langle\Phi_1|\Phi_1\rangle = \sum_{S_z}\left(\frac{d_0^{S_z}}{D_0}\right)^2 (d_1^{S_z})^2, \tag{8}$$

$$|\bar{\phi}_1^{S_z}\rangle = \frac{1}{d_1^{S_z}}|\phi_1\rangle, \quad |\bar{\Phi}_1\rangle = \frac{1}{D_1}|\Phi_1\rangle = \sum_{S_z}\frac{d_0^{S_z}}{D_0}\frac{d_1^{S_z}}{D_1}|\bar{\phi}_1^{S_z}\rangle \tag{9}$$

In general, nth TPQ state are give as follow.

$$|\bar{\Phi}_n\rangle = \sum_{S_z}\left(\prod_{k=0}^{n}\pi_k\right)|\bar{\phi}_n^{S_z}\rangle, \quad \pi_k = \frac{d_k^{S_z}}{D_k}, \tag{10}$$

$$(D_n)^2 = \sum_{S_z}\left(\prod_{k=0}^{n-1}\pi_k\right) \times (d_n^{S_z})^2. \tag{11}$$