Proof of a Possible Form of Green Function on a lattice system

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I. STATEMENT

For a lattice system of any dimension with total size (number of lattice point) L, define annihilation operator as C_i and creation operator as $C_i^\dagger$ for the i-th point. For a single particle, there are L independet eigenstate $|E_k\rangle$, with corresponding eigenenergy E_k. We can write

$$|E_k\rangle = U^{-1}|i\rangle, |i\rangle = U|E_k\rangle, \tag{1}$$

where $|n\rangle$ denotes the occupied state at n-th point. Assume the unitary transformation matrix U takes the form

$$U = \begin{pmatrix} a_{k_1 1} & a_{k_2 1} & \cdots & a_{k_L 1} \\ a_{k_1 2} & a_{k_2 2} & \cdots & a_{k_L 2} \\ \vdots & \ddots & & \\ a_{k_1 L} & a_{k_2 L} & \cdots & a_{k_L L} \end{pmatrix}, \tag{2}$$

and

$$|E_k\rangle = C_k^\dagger|0\rangle, |i\rangle = C_i^\dagger|0\rangle, \tag{3}$$

then the transformations of the annihilation operator and creation operator are

$$C_i = \sum_k a_{ki}C_k, C_i^\dagger = \sum_k a_{ki}^* C_k^\dagger \tag{4}$$

Generally, the Green function for the correlation between the i-th and j-th point can be written as

$$G_{ij} = \left\langle C_i^\dagger C_j \right\rangle. \tag{5}$$

We can PROVE that for an N-particle ground states ($N \leq L$), a possible form of the Green function is

$$G = \begin{pmatrix} a_{k_1 1}^* & a_{k_2 1}^* & \cdots & a_{k_N 1}^* \\ a_{k_1 2}^* & a_{k_2 2}^* & \cdots & a_{k_N 2}^* \\ \vdots & \ddots & & \\ a_{k_1 L}^* & a_{k_2 L}^* & \cdots & a_{k_N L}^* \end{pmatrix}_{L\times N} \begin{pmatrix} a_{k_1 1} & a_{k_1 2} & \cdots & a_{k_1 L} \\ a_{k_2 1} & a_{k_2 2} & \cdots & a_{k_2 L} \\ \vdots & \ddots & & \\ a_{k_N 1} & a_{k_N 2} & \cdots & a_{k_N L} \end{pmatrix}_{N\times L}. \tag{6}$$

II. LEMMA

To prove the statement above, we introduce the Wick's theorem as follow.

$$\langle C_1 C_2 \ldots C_{2N-1} C_{2N}\rangle = \sum_P sgn(P)\langle C_i C_j\rangle\langle C_k C_l\rangle \cdots \langle C_m C_n\rangle, \tag{7}$$

where N is an integer and the right-hand-side of the equation takes the sum of all combinations of expetation value for two operators. $\{i, j, k, l, \cdots, m, n\}$ is any permutation of $\{1, 2, \cdots, 2N-1, 2N\}$, and $sgn(P)$ denotes the sign of the permutation, while the relative position bewteen any annihilation and creation operator pair should be preserved. Here the operators can be annihilation or creation. Obviously for a non-zero result the left-hand-side should be both of number N and any $\langle C_i C_j\rangle$ should contains one annihilation and one creation operator.

For example, if the state is a vaccum state and $N = 2$, the Wick's theorem shows that

$$\left\langle C_1 C_2 C_3^\dagger C_4^\dagger \right\rangle = -\left\langle C_1 C_3^\dagger \right\rangle \left\langle C_2 C_4^\dagger \right\rangle + \left\langle C_1 C_4^\dagger \right\rangle \left\langle C_2 C_3^\dagger \right\rangle, \left\langle C_1 C_2^\dagger C_3 C_4^\dagger \right\rangle = \left\langle C_1 C_2^\dagger \right\rangle \left\langle C_3 C_4^\dagger \right\rangle. \tag{8}$$

III. PROOF

The $N = 1$ case can be easily proved using relations of annihilation and creation operators, without using Wick's Theorem. Now we prove the case for $N = 2$. A two-particle eigenstate can be written as

$$|E\rangle = C^{\dagger}_{k_1} C^{\dagger}_{k_2} |0\rangle . \tag{9}$$

Then the Green function can be wriiten as

$$G_{ij} = \left\langle 0 \left| C_{k_2} C_{k_1} C^{\dagger}_{i} C_j C^{\dagger}_{k_1} C^{\dagger}_{k_2} \right| 0 \right\rangle . \tag{10}$$

After performing unitary transformation on $C^{\dagger}_{i}$ and C_j, that is

$$C_j = \sum_{k'} a_{k'j} C_{k'} , C^{\dagger}_{i} = \sum_{k} a^{*}_{ki} C^{\dagger}_{k}, \tag{11}$$

the Green function becomes

$$G_{ij} = \sum_{kk'} a^{*}_{ki} a_{k'j} \left\langle 0 \left| C_{k_2} C_{k_1} C^{\dagger}_{k} C_{k'} C^{\dagger}_{k_1} C^{\dagger}_{k_2} \right| 0 \right\rangle . \tag{12}$$

Use Wick's theorem and notice the fact that

$$\left\langle 0 \left| C_m C^{\dagger}_{n} \right| 0 \right\rangle = \delta_{mn}, \tag{13}$$

which leads to two zero terms, so

$$\begin{aligned} & \langle 0| C_{k_2} C_{k_1} C^{\dagger}_{k} C_{k'} C^{\dagger}_{k_1} C^{\dagger}_{k_2} |0\rangle \\ = & \langle 0| C_{k_2} C^{\dagger}_{k} |0\rangle \langle 0| C_{k_1} C^{\dagger}_{k_1} |0\rangle \langle 0| C_{k'} C^{\dagger}_{k_2} |0\rangle \\ & + \langle 0| C_{k_2} C^{\dagger}_{k_2} |0\rangle \langle 0| C_{k_1} C^{\dagger}_{k} |0\rangle \langle 0| C_{k'} C^{\dagger}_{k_1} |0\rangle \\ = & \quad \delta_{k_2 k} \delta_{k' k_2} + \delta_{k_1 k} \delta_{k' k_1} . \end{aligned} \tag{14}$$

Thus the Green function becomes

$$G_{ij} = a^{*}_{k_1 i} a_{k_1 j} + a^{*}_{k_2 i} a_{k_2 j}, \tag{15}$$

which can be also written as

$$G = \begin{pmatrix} a^{*}_{k_1 1} & a^{*}_{k_2 1} \\ a^{*}_{k_1 2} & a^{*}_{k_2 2} \\ \vdots & \vdots \\ a^{*}_{k_1 L} & a^{*}_{k_2 L} \end{pmatrix}_{L\times 2} \begin{pmatrix} a_{k_1 1} & a_{k_1 2} & \cdots & a_{k_1 L} \\ a_{k_2 1} & a_{k_2 2} & \cdots & a_{k_2 L} \end{pmatrix}_{2\times L} (QED.). \tag{16}$$

For the cases of $N > 2$, similar process can be followed.