Overcomplete compact representation of susceptibility at a finite bosonic frequency

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I. THE THREE-POINT GREEN'S FUNCTIONS

We consider a three-point Green's function defined by

$$G^{3\mathrm{pt}}(\tau_1,\tau_2,\tau_3) = \langle T_\tau A(\tau_1)B(\tau_2)C(\tau_3)\rangle\,, \tag{1}$$

where A and B are fermionic operators in the Heisenberg picture and C is a bosonic operator. Our expansion formula for $G^{3\mathrm{pt}}$ is

$$\begin{aligned}
&G^{3\mathrm{pt}}(\tau_1,\tau_2,\tau_3)\\
&= \sum_{l_1,l_2=0}^{\infty} \Big\{ G^{(1)}_{l_1 l_2} U^{\mathrm{F}}_{l_1}(\tau_{13}) U^{\mathrm{F}}_{l_2}(\tau_{23})\\
&+ G^{(2)}_{l_1 l_2} U^{\overline{\mathrm{B}}}_{l_1}(\tau_{13}) U^{\mathrm{F}}_{l_2}(\tau_{21}) + G^{(3)}_{l_1 l_2} U^{\mathrm{F}}_{l_1}(\tau_{12}) U^{\overline{\mathrm{B}}}_{l_2}(\tau_{23}) \Big\}.
\end{aligned} \tag{2}$$

$$\begin{aligned}
&G^{3\mathrm{pt}}(i\omega_1, i\omega_2)\\
&\equiv \int_0^\beta d\tau_{13} d\tau_{23} e^{i\omega_1\tau_{13}+i\omega_2\tau_{23}} G^{3\mathrm{pt}}(\tau_1,\tau_2,\tau_3)\\
&= \sum_{l_1,l_2=0}^{\infty} \Big\{ G^{(1)}_{l_1 l_2} U^{\mathrm{F}}_{l_1}(i\omega_1) U^{\mathrm{F}}_{l_2}(i\omega_2)\\
&\quad + G^{(2)}_{l_1 l_2} U^{\overline{\mathrm{B}}}_{l_1}(i\omega_1+i\omega_2) U^{\mathrm{F}}_{l_2}(i\omega_2)\\
&\quad + G^{(3)}_{l_1 l_2} U^{\mathrm{F}}_{l_1}(i\omega_1) U^{\overline{\mathrm{B}}}_{l_2}(i\omega_1+i\omega_2) \Big\}.
\end{aligned} \tag{3}$$

II. THE FOUR-POINT GREEN'S FUNCTIONS

$$\begin{aligned}
&G^{4\mathrm{pt}}(\tau_1,\tau_2,\tau_3,\tau_4)\\
&= \sum_{l_1,l_2,l_3=0}^{\infty} \Big\{ G^{(1)}_{l_1 l_2 l_3} U^{\mathrm{F}}_{l_1}(\tau_{14}) U^{\mathrm{F}}_{l_2}(\tau_{24}) U^{\mathrm{F}}_{l_3}(\tau_{34})\\
&\qquad + \cdots\\
&\qquad + G^{(16)}_{l_1 l_2 l_3} U^{\mathrm{F}}_{l_1}(\tau_{32}) U^{\overline{\mathrm{B}}}_{l_2}(\tau_{21}) U^{\mathrm{F}}_{l_3}(\tau_{14}) \Big\}\\
&\equiv \sum_{r=1}^{16} \sum_{l_1,l_2,l_3=0}^{\infty} G^{(r)}_{l_1 l_2 l_3} U^{\alpha}_{l_1}(\tau) U^{\alpha'}_{l_2}(\tau') U^{\alpha''}_{l_3}(\tau''),
\end{aligned} \tag{4}$$

$$\chi(\tau_{12},\tau_{34},i\omega_m) \equiv \int_0^\beta d\tau_1 G^{4\mathrm{pt}}(\tau_1,\tau_2,\tau_3,0) e^{i\omega_m\tau_1} \tag{5}$$

The dependency on two fermionic frequencies at a fixed bosonic frequency is represented as

$$\begin{aligned}
&\chi(\tau_{12},\tau_{34},i\omega_m)\\
&= \sum_{s,s'=0,1} \sum_{l_1,l_2=0}^{\infty} \Big\{ G^{(1)}_{ss' l_1 l_2} U^{\mathrm{F}}_{s l_1}(\tau_{12}) U^{\mathrm{F}}_{s' l_2}(\tau_{34})\\
&+ G^{(2)}_{ss' l_1 l_2} U^{\overline{\mathrm{B}}}_{s l_1}(\tau_{12}) U^{\mathrm{F}}_{s' l_2}((-1)^{s'}\tau_{12}+\tau_{34})\\
&+ G^{(3)}_{ss' l_1 l_2} U^{\overline{\mathrm{B}}}_{s l_1}(\tau_{34}) U^{\mathrm{F}}_{s' l_2}(\tau_{12}+(-1)^{s'}\tau_{34}) \Big\}.
\end{aligned} \tag{6}$$

$$U^{\alpha}_{sl}(\tau) \equiv e^{is\omega_m\tau} U^{\alpha}_{l}(\tau). \tag{7}$$

In the Matsubara domain, this reads

$$\begin{aligned}
&\chi(i\omega_n, i\omega_{n'}, i\omega_m)\\
&\equiv \int_0^\beta d\tau_{12} d\tau_{34} e^{i\omega_n\tau_{12}+i\omega_{n'}\tau_{34}} \chi(\tau_{12},\tau_{34},i\omega_m)\\
&\equiv \int_0^\beta d\tau_{12} d\tau_{34} d\tau_{14} e^{i\omega_n\tau_{12}+i\omega_{n'}\tau_{34}+i\omega_{n'}\tau_{14}} G^{3\mathrm{pt}}(\tau_1,\tau_2,\tau_3,\tau_4)\\
&= \sum_{s,s'=0,1} \sum_{l_1,l_2=0}^{\infty} \Big\{ G^{(1)}_{ss' l_1 l_2} U^{\mathrm{F}}_{s l_1}(i\omega_n) U^{\mathrm{F}}_{s' l_2}(i\omega_{n'})\\
&\quad + G^{(2)}_{ss' l_1 l_2} U^{\overline{\mathrm{B}}}_{l_1 s}(i\omega_n + (-1)^{s+1} i\omega_{n'}) U^{\mathrm{F}}_{l_2 s'}(i\omega_{n'})\\
&\quad + G^{(3)}_{ss' l_1 l_2} U^{\overline{\mathrm{B}}}_{l_1 s}(i\omega_{n'} + (-1)^{s+1} i\omega_n) U^{\mathrm{F}}_{l_2 s'}(i\omega_n) \Big\}.
\end{aligned} \tag{8}$$

$$U^{\alpha}_{sl}(i\omega_n) \equiv U^{\alpha}_{l}(i\omega_n + s i\omega_m) \tag{9}$$

III. TENSOR REGRESSION

We decomposed the particle-hole view of the two-particle Green's function as

$$G(r,l_1,l_2) = \sum_{d=1}^{D} C(d,r) X_1(d,l_1) X_2(d,l_2), \tag{10}$$

where r is the index of 12=($3\times 2\times 2$) orthogonal systems. This is referred to as a CP decomposition [canonical (CANDECOMP) / parallel pactors (PARAFAC)]. We will find useful information in "Tensor Learning for Regression" written by Weiwei Guo, Irene Kotsia.

The cost function reads

$$\begin{aligned}
&|G(\boldsymbol{n}) - U(\boldsymbol{n},r,l_1)U(\boldsymbol{n},r,l_2)G(r,l_1,l_2)|_2^2\\
&\qquad + \alpha\left\{|C|_2^2 + |X_1|_2^2 + |X_2|_2^2\right\},
\end{aligned} \tag{11}$$

where $\boldsymbol{n} \equiv (n, n', m)$ runs over sampling points in the Matsubara frequency domain. This cost function can be minimized using alternative projections since the penalty term is separable with respect to C, X_1 or X_2. That is,

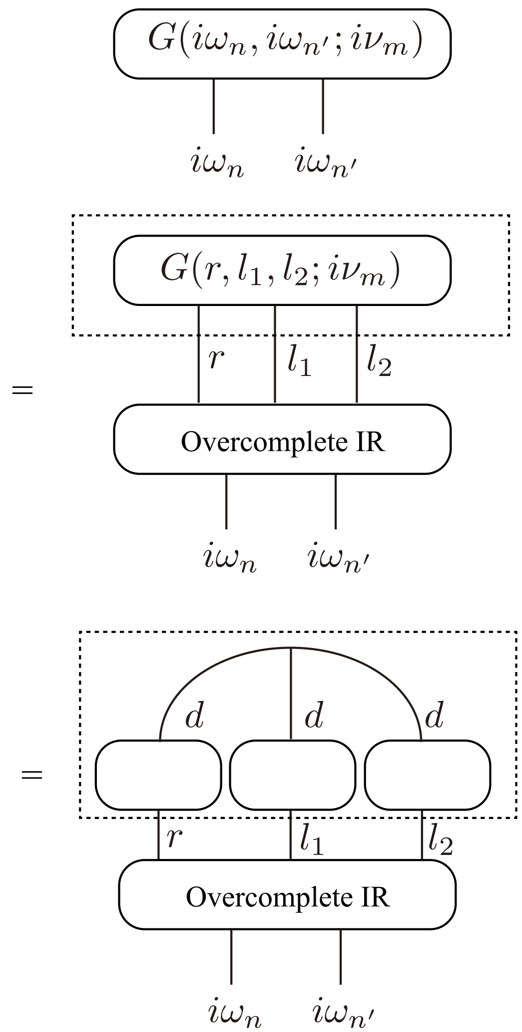

FIG. 1. Graphical representation of CP decomposition

we minimize the cost function with respect to either C, X_1 or X_2 at one time. This ends up with performing many smaller Ridge regressions.