Dynamical mean-field approach to Ising models with impurities

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Abstract

This article comprises of four parts. First, it presents the essentials of DMFT algorithms in classical Euclidean field theory, with Gibbs measure and Ising models. Second, it discusses an approximation method to the interacting particles. Third, it investigates an extended impurity problem. The Legendre dual correspondence, properties and formalism of Luttinger-Ward functional, and Φ-derivability of physical quantities are proposed and verified. Finally, this article ends with a revised iterative DMFT to compute this extended model.

1 Introduction

Traditionally, Feynman's diagrammatic expansion of many-body perturbation theory provides an universal method to compute physical quantities [2] in any statistical systems [4, 10]. But such diagrammatic expansions are, unfortunately, only formal. On the one hand, divergence and renormalization destroys the strictness of mathematics. On the other hand, applying this method to extremely large systems in statistical mechanics becomes impossible, see also [11].

However, we could still extract information from this model (*i.e.* Gibbs measure) by omitting weak interactions between clusters among the particles. Then we give the local Gibbs measures and tensoring them in the hope that we retrieve the original local Green's functions and first moments. The methods we adopt is the DMFT algorithms that we introduce the following sections. For an exposition in this direction, see [3, 12].

2 Basic Settings

Let $M = RL$, $x_c = (x_{(c-1)L+1}, \ldots, x_{cL})$ and define the generalized interaction measure

$$\mathrm{d}\mu(x) = e^{-\frac{1}{2}x^T Ax} \prod_{c=1}^{R} \sum_{\sigma\in\{-1,1\}^L} \mathrm{d}\delta(x_c - \sigma)$$

where $\mathrm{d}\mu(x)$ specifies the global setting. and the partition function

$$Z = \int_{\mathbb{R}^M} \mathrm{d}\mu(x)$$

Theoretically, we could also attempt to compute the global Green's correlator function $G \in \mathbb{R}^{M\times M}$

$$G = \left\langle xx^T \right\rangle_\mu = \frac{1}{Z}\int_{\mathbb{R}^M} xx^T \mathrm{d}\mu(x)$$

But we want to avoid this tremendous computation [6], and approximate this global Ising model into local impurities. In other words, we define the measure $\mathrm{d}\mu_c(x_c)$, $c = 1, \dots, R$ on $\mathbb{R}^L$ for each impurity such that

$$\mathrm{d}\mu(x) \approx \mathrm{d}\mu_1(x_1) \otimes \cdots \otimes \mathrm{d}\mu_R(x_R)$$

in the sense that we retrive each of the c^{th} diagonal $L \times L$ block in the original Green's function with $\mathrm{d}\mu_c(x_c)$. Hence, for each $c = 1, \dots, R$, in principle, we want to find $\Delta_c \in \mathbb{R}^{L\times L}$ such that

$$\mathrm{d}\mu_c(x_c) = e^{-\frac{1}{2}x_c^T(A_c+\Delta_c)x_c} \sum_{\sigma\in\{-1,1\}^L} \mathrm{d}\delta(x_c - \sigma)$$

Notice that we call $\Delta_c \in \mathbb{R}^{L\times L}$ the exact hybridization, with which we retrive the original c^{th} block of the global Green's function in $\mathbb{R}^{M\times M}$. Hence, our aim is to choose Δ_c such that

$$G_c = G[\mathrm{d}\mu_c(x_c)] = G[\mathrm{d}\mu(x)]_c$$

where

$$G_c = \left\langle x_c x_c^T \right\rangle_{\mathrm{d}\mu_c} = \sum_{\sigma\in\{-1,1\}^L} \sigma\sigma^T e^{-\frac{1}{2}\sigma(A_c+\Delta_c)\sigma^T} \Bigg/ \sum_{\sigma\in\{-1,1\}^L} e^{-\frac{1}{2}\sigma(A_c+\Delta_c)\sigma^T}$$

This computation is confined in the $L \times L$ case, which makes life easier. And we could use Metropolis algorithm to numerically solve G_c once we know Δ_c.

3 Introducing DMFT Algorithms

In order to compute $\Delta_c \in \mathbb{R}^{L\times L}$, we use DMFT algorithm. First, we choose the initial value

$$\Delta_c^{(0)} = 0$$

Then the initial impurity measure

$$\mathrm{d}\mu_c^{(0)}(x_c) = e^{-\frac{1}{2}x_c^T A_c x_c} \sum_{\sigma\in\{-1,1\}^L} \mathrm{d}\delta(x_c - \sigma)$$

And the initial c^{th} impurity partition function

$$Z_c^{(0)} = \int_{\mathbb{R}^L} \mathrm{d}\mu_c^{(0)}(x_c) = \sum_{\sigma\in\{-1,1\}^L} e^{-\frac{1}{2}\sigma^T A_c \sigma}$$

And then follows the initial c^{th} block Green's function

$$G_c^{(0)} = \left\langle x_c x_c^T \right\rangle_{\mu_c} = \sum_{\sigma\in\{-1,1\}^L} \sigma\sigma^T e^{-\frac{1}{2}\sigma A_c \sigma^T} \Bigg/ \sum_{\sigma\in\{-1,1\}^L} e^{-\frac{1}{2}\sigma A_c \sigma^T}$$

Since $A_c + \Delta_c^{(0)} = A_c \longleftrightarrow \Sigma_c^{(0)}$ via Legendre correspondence, we have

$$\Sigma_c^{(0)} = A_c + \Delta_c^{(0)} - (G_c^{(0)})^{-1}$$

by Dyson's equation. Then we use the direct sum of $\{\Sigma_c^{(0)}; c = 1, \dots, R\}$ as an ansatz for the self-energy of the original Ising model

$$\Sigma^{(0)} = \bigoplus_{1\leq c\leq R} \Sigma_c^{(0)}[A_c + \Delta_c^{(0)}]$$

Then by the Dyson's equation for the global setting, we have

$$G^{(0)} = (A + \Lambda^{(0)} - \Sigma_c^{(0)})^{-1}$$

Notice that theoretically $\Lambda^{(0)} \in \mathbb{R}^{M\times M}$ should vanish. But we want a better approximation. Considering that the global setting satisfies $\text{diag}(G) = Id_M$, we could implement $\Lambda^{(0)} = \text{diag}(\lambda^{(0)})$ and $\text{diag}(G^{(0)}) = \text{diag}((A + \Lambda^{(0)} - \Sigma_c^{(0)})^{-1}) = Id_M$.

Then, let $\pi_c : \mathbb{R}^M \mapsto \mathbb{R}^L$ be the canonical projection map onto c^{th} L-dimensional subspace. We have

$$\Delta_c^{(1)} = \Sigma_c^{(0)} - A_c + (\pi_c G^{(0)} \pi_c^T)^{-1}$$

Hence the iteration continues and $\forall n \in \mathbb{N}$,

$$G_c^{(n)} = \left\langle x_c x_c^T \right\rangle_{\mu_c^n} = \sum_{\sigma\in\{-1,1\}^L} \sigma\sigma^T e^{-\frac{1}{2}\sigma(A_c+\Delta_c^{(n)})\sigma^T} \Bigg/ \sum_{\sigma\in\{-1,1\}^L} e^{-\frac{1}{2}\sigma(A_c+\Delta_c^{(n)})\sigma^T}$$

And the self-energy,

$$\Sigma_c^{(n)} = A_c + \Delta_c^{(n)} - (G_c^{(n)})^{-1}$$

$$\Sigma^{(n)} = \bigoplus_{1\le c\le R} \Sigma_c^{(n)}$$

And the global Green's function,

$$G^{(n)} = (A + \Lambda^{(n)} - \Sigma^{(n)})^{-1}$$

And the exact hybridization,

$$\Delta_c^{(n+1)} = \Sigma_c^{(n)} - A_c + (\pi_c G^{(n)} \pi_c^T)^{-1}$$

where $\Lambda^{(n)} \in \mathbb{R}^{M\times M}$, $\Lambda^{(n)} = \text{diag}(\lambda^{(n)})$ are similarly defined as $\Lambda^{(0)}$ to ensure that $\text{diag}(G^{(n)}) = Id_M$. Notice that we could use Metropolis algorithm to solve explicitly for $\Lambda^{(n)}$ once we are fully convinced that a unique $\Lambda^{(n)} = \text{diag}(\lambda^{(n)})$ exists.

Notice that $\forall n \in \mathbb{N}$, $G^{(n)} = (A + \Lambda^{(n)} - \Sigma^{(n)})^{(-1)}$. Hence, we know

$$\begin{aligned}
\text{diag}(G^{(n)}) - Id_M &= \text{diag}((A + \Lambda^{(n)} - \Sigma^{(n)})^{-1}) - Id_M \\
&= \text{diag}((A - \Sigma^{(n)} + \text{diag}(\lambda^{(n)}))^{-1}) - Id_M \\
&= \nabla f_n(\lambda^{(n)})
\end{aligned}$$

where

$$f_n(\lambda^{(n)}) = \log\det\Big(A - \Sigma^{(n)} + \text{diag}(\lambda^{(n)})\Big) - \sum_{1\le i\le M} \lambda_i^{(n)}$$

Since the map $\lambda^{(n)} \mapsto \sum_{1\le i\le M} \lambda_i^{(n)}$ is convex, and since the map $\lambda^{(n)} \mapsto \log\det\big(A - \Sigma^{(n)} + \text{diag}(\lambda^{(n)})\big)$ is strictly concave on its domain $\{\lambda^{(n)} \in \mathbb{R}^M; \det\big(A - \Sigma^{(n)} + \text{diag}(\lambda^{(n)})\big) > 0\}$, which is a convex set in $\mathbb{R}^M$. Therefore, we could say there is at most one unique maximizer (also denoted as $\lambda^{(n)}$) of $f_n : \mathbb{R}^M \to \mathbb{R}$. Since the smoothness of $f_n(\lambda^{(n)})$ is obvious, we know immediately that $\text{diag}(G^{(n)}) - Id_M = \nabla f_n(\lambda^{(n)}) = 0$ becasue a maximizer is always a stationary point.

4 Interaction Potential Approximation

The Ising model incorporates measure μ and μ_c respectively on $\mathbb{R}^M$ and $\mathbb{R}^L$, which are not absolutely continuous with respect to the Lebesgue measure [7]. And this singularity prevents us from using ordinary methods discussed in the dissertation paper. Hence, we want to find a way to approximate the local singular measure μ_c with a measure $\eta_{c,\alpha}$ on $\mathbb{R}^L$, parametrized by $\alpha > 0$, which is absolutely continuous with respect to the Lebesgue measure. This section proceeds the previous work of [13].

For $\forall n \in \mathbb{N}$, we have

$$\mathrm{d}\mu_c^{(n)}(x_c) = e^{-\frac{1}{2}x_c^T(A_c+\Delta^{(n)})x_c} \sum_{\sigma\in\{-1,1\}^L} \mathrm{d}\delta(x_c-\sigma)$$

We choose

$$U_c(x_c) = \frac{1}{8}\sum_{i,j=1}^{L} v_{ij}(x_i^2-1)(x_j^2-1) = \frac{1}{4}\sum_{i,j=1}^{L} \delta_{ij}(x_i^2-1)(x_j^2-1)$$

This is the interacting potential energy what we will use to approximate the measure μ_c. Then, define

$$\mathrm{d}\eta_{c,\alpha}^{(n)}(x_c) = e^{-\frac{1}{2}x_c^T(A_c+\Delta_c^{(n)})x_c-\alpha U_c(x_c)}\mathrm{d}x_c$$

Notice that $\mathrm{d}\eta_{c,\alpha}^{(n)}(x_c) \to \mathrm{d}\mu_c^{(n)}(x_c)$ weakly as $\alpha \to \infty$. Therefore, any proper integral with respect to $\mathrm{d}\eta_{c,\alpha}^{(n)}$ converges to its integral with respect to $\mathrm{d}\mu_c^{(n)}$ in $\mathbb{R}$ because of the weak convergence.

Now choose $\alpha > 0$ large enough. We know that $\alpha U_c(x_c)$ satisfies the strong growth condition. Hence $\operatorname{dom}\Omega_c^{(n)} = \mathcal{S}^L$. Moreover, we have the Legendre correspondence $A_c + \Delta_c^{(n)} \longleftrightarrow G_{c,\alpha}^{(n)}$ under the potential energy $\alpha U_c(x_c)$, where $G_{c,\alpha}^{(n)} = \left\langle x_c x_c^T \right\rangle_{\eta_{c,\alpha}^{(n)}}$ And by the above discussed weak convergence of measures, we are confident that

$$\lim_{\alpha\to\infty} G_{c,\alpha}^{(n)} = G_c^{(n)}$$

where $G_c^{(n)}$ is the local Green's function for $\mu_c^{(n)}$ discussed above.

5 Adding a Linear Term

When $\mathcal{H}(x) = \frac{1}{2}x^*Ax + a^*x + U(x)$, where $U(x)$ satisfies the weak growth condition, we have

$$Z[A,a] = \int e^{-\mathcal{H}(x)}\mathrm{d}x$$

$$\Omega[A,a] = -\log Z[A,a]$$

$$G[A,a] = \langle xx^*\rangle = \frac{1}{Z[A,a]}\int xx^* e^{-\mathcal{H}(x)}\mathrm{d}x$$

$$g[A,a] = \langle x\rangle = \frac{1}{Z[A,a]}\int x e^{-\mathcal{H}(x)}\mathrm{d}x$$

We want to compute the self energy $\Sigma[G,g]$ and $\sigma[G,g]$ such that the probability measure $\mathrm{d}\mu \sim e^{\frac{1}{2}x^*(A-\Sigma)x-(a-\sigma)^*x}\mathrm{d}x$ modulo normalization, up to the same second moments G and first moments g with the probability measure $\frac{1}{Z[A,a]}e^{-\mathcal{H}(x)}\mathrm{d}x$.

Notice that $\mathrm{d}\mu$ turns out to be a Gaussian and hence $\mathrm{d}\mu \sim e^{-\frac{1}{2}(x-g)^*(G-gg^*)^{-1}(x-g)}\mathrm{d}x$. Therefore, through matrix algebra, we calculate $\Sigma = A - (G-gg^*)^{-1}$ and $\sigma = a + (G-gg^*)^{-1}g$, see [14]. We want to consider the transformation rule for this setting $\frac{1}{Z[A,a]}e^{-\mathcal{H}(x)}\mathrm{d}x$, but we need to define some corresponding physical quantities first.

Define $\mathcal{G} : \mathcal{M}_1 \cap \mathcal{M}_2 \to \mathcal{S}_+^N$ such that $\mathcal{G}(\mu) = \int xx^* \mathrm{d}\mu$, which is specification of second moment. Define $\mathcal{P} : \mathcal{M}_1 \cap \mathcal{M}_2 \to \mathbb{R}^N$ such that $\mathcal{P}(\mu) = \int x \mathrm{d}\mu$, which is the specification of first moments. Notice that the Legendre dual

$$\mathcal{F}[G,g] = \sup_{\mu \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[H(\mu) - \int U \mathrm{d}\mu \right]$$

where $H(\mu)$ denotes the differential entropy, and hence we have

$$\mathcal{F}[G,g] = \sup_{\mu \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[-\int \log\left(\frac{\mathrm{d}\mu}{\mathrm{d}\lambda}\right) \mathrm{d}\mu - \int U \mathrm{d}\mu \right]$$

where $\mathrm{d}\lambda$ refers to the Lebesgue measure.

When $U \equiv 0$, we have $\mathcal{F}[G,g] = \sup_{\mu \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} H(\mu)$. Notice that the random variable X achieving the maximal differential entropy such that $\mathbb{E}[X_i X_j] = G_{ij}$ and $\mathbb{E}[X_i] = g_i$ follows a Gaussian distribution, i.e. $X \sim \mathcal{N}(g, G - gg^*)$. Hence,

$$\mathcal{F}[G,g] = \frac{1}{2} \operatorname{Tr}[\log(G - gg^*)] + \frac{N}{2} \log(2\pi e)$$

. Then, for general $U : \mathbb{R}^N \to \mathbb{R}$, we define the Luttinger Ward functional

$$\Phi[G,g,U] = 2\mathcal{F}[G,g] - \operatorname{Tr}[\log(G - gg^*)] - N \log(2\pi e)$$

Going back to the definition of $\mathcal{F}$, we express Φ as

$$\begin{aligned}
\Phi[G,g,U] &= -N \log(2\pi e) - \log[\det(G - gg^*)] + 2 \sup_{\mu \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[H(\mu) - \int U \mathrm{d}\mu \right] \\
&= -N \log(2\pi e) - \log[\det(G - gg^*)] - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[\int (\log(\rho) + U) \rho \mathrm{d}x \right] \\
&= -N \log(2\pi e) - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[\int (\log[(\det G - gg^*)^{1/2} \rho] + U) \rho \mathrm{d}x \right]
\end{aligned}$$

Let $C = -N \log(2\pi e)$, then we want to formulate the transformation rule for the setting $e^{-\mathcal{H}(x)} \mathrm{d}x$. Suppose $T : \mathbb{R}^N \to \mathbb{R}^N$ is a linear isomorphism. Then

$$\begin{aligned}
\Phi[TGT^*, Tg, U] &= C - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(TGT^*) \cap \mathcal{P}^{-1}(Tg)} \left[\int (\log[(\det TGT^* - Tgg^*T*)^{1/2} \cdot \rho] + U) \rho \mathrm{d}x \right] \\
&= C - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(TGT^*) \cap \mathcal{P}^{-1}(Tg)} \left[\int (\log[(\det G - gg^*)^{1/2} \cdot |\det T| \cdot \rho] + U) \rho \mathrm{d}x \right]
\end{aligned}$$

Consider the change of variable:

$$\begin{aligned}
\{\rho : \rho \mathrm{d}x \in \mathcal{G}^{-1}(TGT^*) \cap \mathcal{P}^{-1}(Tg)\} &= \{\rho : |\det T| \cdot \rho \circ T \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)\} \\
&= \{|\det T|^{-1} \cdot \rho \circ T^{-1} : \rho \mathrm{d}x \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)\}
\end{aligned}$$

Because $\rho \mathrm{d}x \in \mathcal{G}^{-1}(TGT^*) \iff \int xx^* \rho \mathrm{d}x = TGT^* \iff \int Tyy^*T^* \rho(Ty) |\det T| \mathrm{d}y = TGT^*$, where we let $x = Ty \iff |\det T| \cdot \rho \circ T \in \mathcal{G}^{-1}(G)$. Similarly, we know $\rho \mathrm{d}x \in \mathcal{P}^{-1}(Tg) \iff \int x \rho \mathrm{d}x = Tg \iff \int Ty \rho(Ty) |\det T| \mathrm{d}y = Tg$, where we let $x = Ty \iff |\det T| \rho \circ T \in \mathcal{P}^{-1}(g)$. Hence we have verified that

$$\{\rho : \rho \mathrm{d}x \in \mathcal{G}^{-1}(TGT^*) \cap \mathcal{P}^{-1}(Tg)\} = \{|\det T|^{-1} \cdot \rho \circ T^{-1} : \rho \mathrm{d}x \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)\}$$

Hence,

$$\begin{aligned}
\Phi[TGT^*, Tg, U] &= C - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(TGT^*) \cap \mathcal{P}^{-1}(Tg)} \left[\int (\log[(\det G - gg^*)^{1/2} \cdot |\det T| \cdot \rho] + U)\rho \mathrm{d}x \right] \\
&= C - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[|\det T|^{-1} \int (\log[(\det G - gg^*)^{1/2} \cdot \rho \circ T^{-1}] + U)\rho \circ T^{-1} \mathrm{d}x \right] \\
&= C - 2 \inf_{\rho \mathrm{d}x \in \mathcal{G}^{-1}(G) \cap \mathcal{P}^{-1}(g)} \left[\int (\log[(\det G - gg^*)^{1/2} \cdot \rho] + U \circ T)\rho \mathrm{d}x \right] \\
&= \Phi[G, g, U \circ T]
\end{aligned}$$

Hence we have verified the transformation rule for Luttinger Ward functional in this setting.

Before investigating the sparsity patterns of impurity models, we present a natural consequence of the first moments.

Consider $U\mathbb{R}^p \to \mathbb{R}$, depending only on the first p variables. Then,

$$\begin{aligned}
g_2 &= \frac{1}{Z} \int x_2 e^{-\mathcal{H}(x)} \mathrm{d}x \\
&= \frac{1}{Z} \iint x_2 e^{-\frac{1}{2}x^* A x - a^* x - U(x_1)} \mathrm{d}x_1 \mathrm{d}x_2 \\
&= \frac{1}{Z} \iint x_2 e^{-\frac{1}{2}x_1^* A_{11} x_1 - a_1^* x_1 - U(x_1)} \mathrm{d}x_1 e^{\frac{1}{2}(a_2 + A_{21}x_1)^* A_{22}^{-1}(a_2 + A_{21}x_1)} e^{-\frac{1}{2}y_2^* A_{22} y_2} \mathrm{d}y_2
\end{aligned}$$

where $y_2 = x_2 + A_{22}^{-1}(a_2 + A_{21}x_1)$ and $x_2 = y_2 - A_{22}^{-1}(a_2 + A_{21}x_1)$. Then,

$$\begin{aligned}
\frac{1}{Z} \int x_2 e^{-\mathcal{H}(x)} \mathrm{d}x &= \frac{1}{Z} \iint y_2 e^{-\frac{1}{2}y_2^* A_{22} y_2} \mathrm{d}y_2 \mathrm{d}x_1 \\
&\quad - \frac{1}{Z} \iint A_{22}^{-1}(a_2 + A_{21}x_1) e^{-\frac{1}{2}x_1^* A_{11} x_1 - a_1^* x_1 - U(x_1)} e^{\frac{1}{2}(a_2 + A_{21}x_1)^* A_{22}^{-1}(a_2 + A_{21}x_1)} \mathrm{d}x_1 \mathrm{d}y_2 \\
&= -A_{22}^{-1}(a_2 + A_{21}g_1)
\end{aligned}$$

Hence, $A_{22}g_2 + A_{21}g_1 + a_2 = 0$. Notice this result is quite consistent with the two known scenarios where $U : \mathbb{R}^N \to \mathbb{R}$ and $U \equiv 0$. In the first case, everything on the left-hand side vanishes. In the second case, $A = A_{22}$ and we have $g = g_2$, $e^{-\mathcal{H}(x)}\mathrm{d}x \sim e^{-\frac{1}{2}x^x Ax - a^* x}\mathrm{d}x \sim \mathcal{N}(-A^{-1}a, A^{-1})$.

Now we come back to discuss the sparsity properties of the impurity model $U : \mathbb{R}^p \to \mathbb{R}$. We have verified the transformation rule that $\forall T \in GL_n(\mathbb{R}) \Longrightarrow \Phi[TGT^*, Tg, U] = \Phi[G, g, U \circ T]$.

As for the projection rule, we cannot brutally apply the canonical projection map $\pi : \mathbb{R}^N \to \mathbb{R}^p$ to the transformation rule. It is routine to give a rigorous but lengthy proof, but an intuitive reasoning may be more appealing. In a word, we could imagine there is a sequence of linear invertible maps $\{T_k : k \in \mathbb{N}\} \subseteq GL_n(\mathbb{R})$ such that $T_k \to \pi$ is a proper sense of metric. Notice that the limit, if exists, must be unique, since $GL_n(\mathbb{R})$ is a Hausdorff space. Intuitively, we have

$$\Phi[\pi G \pi^*, \pi g, U] = \lim_{k \to \infty} \Phi[T_k G T_k^*, T_k g, U] = \lim_{k \to \infty} \Phi[G, g, U \circ T_k] = \Phi[G, g, U \circ \pi]$$

Hence, $\Phi_N[G, g, U] = \Phi_p[G_{11}, g_1, U]$ given that $U : \mathbb{R}^N \to \mathbb{R}$.

The above paragraph provides intuition to understand the projection rule via an informal application of the transformation rule. However, a more rigorous proof is presented below to complete the picture. Since $(G - gg^*) \in \mathcal{S}_{++}^N$ and $gg^* \in \mathcal{S}_+^*$, we know $G \in \mathcal{S}_{++}^*$. And write

$$G = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}$$

we know G_{11} is invertible and define

$$T = \begin{pmatrix} Id & 0 \\ G_{21}G_{11}^{-1} & Id \end{pmatrix}, \quad \widetilde{G} = \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} - G_{21}G_{11}^{-1}G_{12} \end{pmatrix}, \quad \widetilde{g} = \begin{pmatrix} g_1 \\ g_2 - G_{21}G_{11}^{-1}g_1 \end{pmatrix}$$

Then, $T\widetilde{G}T^* = G$ and $T\widetilde{g} = g$. Hence, via transformation rule,

$$\Phi_N[G, g, U] = \Phi_N[\widetilde{G}, \widetilde{g}, U \circ T] = \Phi_N[\widetilde{G}, \widetilde{g}, U]$$

since $U : \mathbb{R}^p \to \mathbb{R}$ depends only on the first p variables. Notice that $\widetilde{G}$ is block-diagonal with the same upper left block as G, and $\widetilde{g}$ has the same first p entries as g, we could consider block-diagonal second moments cases. So now we assume that $G \in \mathcal{S}_{++}^N$ with

$$G = \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix}, \quad g = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$$

Recall the expression for the dual,

$$\mathcal{F}_N[G, g, U] = \sup_{\mu \in \mathcal{G}_N^{-1}(G) \cap \mathcal{P}_N^{-1}(g)} \left[H(\mu) - \int U \mathrm{d}\mu \right]$$

Next we define $\pi_1 : \mathbb{R}^N \to \mathbb{R}^p$ and $\pi_2 : \mathbb{R}^N \to \mathbb{R}^q$ to be the projections onto the first p and last q components, where $q = N - p$, respectively. Then, with $\pi_1 \# \mu$ and $\pi_2 \# \mu$ being the marginals of μ with respect to the product $\mathbb{R}^N = \mathbb{R}^p \times \mathbb{R}^q$. Recall the inequality for differential entropy $H(\mu) \leq H(\pi_1 \# \mu) + H(\pi_2 \# \mu)$. Also notice that $\pi_1 \# \mu \in \mathcal{G}_p^{-1}(G_{11}) \cap \mathcal{P}_p^{-1}(g_1)$ provided that $\mu \in \mathcal{G}_N^{-1}(G) \cap \mathcal{P}_N^{-1}(g)$. Finally, with $U : \mathbb{R}^p \to \mathbb{R}$, we know $\int U \mathrm{d}\mu = \int U \mathrm{d}(\pi_1 \# \mu)$

Then,

$$\begin{aligned}
\mathcal{F}_N[G, g, U] &\leq \sup_{\mu \in \mathcal{G}_N^{-1}(G) \cap \mathcal{P}_N^{-1}(g)} \left[H(\pi_1 \# \mu) + H(\pi_2 \# \mu) - \int U \mathrm{d}(\pi_1 \# \mu) \right] \\
&\leq \sup_{\mu_1 \in \mathcal{G}_p^{-1}(G_{11}) \cap \mathcal{P}_p^{-1}(g_1)} \left[H(\mu_1) - \int U \mathrm{d}\mu_1 \right] + \sup_{\mu_2 \in \mathcal{G}_q^{-1}(G_{22}) \cap \mathcal{P}_q^{-1}(g_2)} H(\mu_2) \\
&= \mathcal{F}_p[G_{11}, g_1, U] + \frac{1}{2} \log \left((2\pi e)^{N-p} \det G_{22} \right)
\end{aligned}$$

where $\det G = \det G_{11} \det G_{22}$. Hence,

$$\Phi_N[G, g, U] \leq \Phi_p[G_{11}, g_1, U]$$

Conversely, $\forall \mu_1 \in \mathcal{G}_p^{-1}(G_{11}) \cap \mathcal{P}_p^{-1}(g_1)$, choose $\mu_2 \in \mathcal{N}(0, G_{22})$ and choose $\mathrm{d}\mu = \mathrm{d}\mu_1 \otimes \mathrm{d}\mu_2$. Then,

$$\mathcal{F}_N[G, g, U] \geq H(\mu) - \int U \mathrm{d}\mu = H(\mu_1) - \int U \mathrm{d}\mu_1 + \frac{1}{2} \log \left((2\pi e)^{N-p} \det G_{22} \right)$$

Since μ_1 is arbitrary in $\mathcal{G}_p^{-1}(G_{11}) \cap \mathcal{P}_p^{-1}(g_1)$, we take the supremum over μ_1 and

$$\mathcal{F}_N[G, g, U] \geq \mathcal{F}_p[G_{11}, g_1, U] + \frac{1}{2} \log \left((2\pi e)^{N-p} \det G_{22} \right)$$

Hence,

$$\Phi_N[G, g, U] \geq \Phi_p[G_{11}, g_1, U]$$

which proves the quality and verifies the projection rule.

Here we comes to our result of sparsity pattern, the formalism of self energy.

$$\Sigma_N[G, g, U] = \frac{1}{2}\nabla\phi_N[G, g, U] = \begin{pmatrix} \Sigma_p[G_{11}, g_1, U] & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\begin{aligned}
\sigma_N[G, g, U] &= a + G^{-1}g \\
&= a + (A - \Sigma_N)g \\
&= \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} + \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{pmatrix} \begin{pmatrix} g_1 \\ -A_{22}^{-1}(a_2 + A_{21}g_1) \end{pmatrix} + \begin{pmatrix} \Sigma_p & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} g_1 \\ A_{22}^{-1}(a_2 + A_{21}g_1) \end{pmatrix} \\
&= \begin{pmatrix} \sigma_p \\ 0 \end{pmatrix}
\end{aligned}$$

where $\sigma_p = a_1 + (A_{11} - A_{12}A_{22}^{-1}A_{21} + \Sigma_p)g_1 - A_{12}A_{22}^{-1}a_2$. Hence we have verified the sparsity pattern for this setting.

Notice that the above discussion of the sparsity patterns of self energies follows a rather conceptual approach. And we may switch to another avenue which involves more computations. Remember that $\Sigma = A - (G - gg^*)^{-1}$ and $\sigma = a + (G - gg^*)^{-1}g$.

For the sparsity pattern of Σ, we want to show that $\Sigma_{12} = 0$, $\Sigma_{21} = 0$, and $\Sigma_{22} = 0$. We could show that $(G - gg^*)^{-1}_{22} = A_{22}$ and $(G - gg^*)^{-1}_{12} = A_{12}$. Notice that $\Sigma_{12} = 0$ *iff* $\Sigma_{21} = 0$. Equivalently, by multiplying both sides by $(G - gg^*)$, we need to show that $[(G - gg^*)A]_{12} = 0_{p\times q}$ and $[(G - gg^*)A]_{22} = Id_q$.

Notice that $(G - gg^*)A = \langle xx^* - gg^* \rangle A$, and

$$[(xx^* - gg^*)A]_{12} = \left[x_1 \begin{pmatrix} x_1^* & x_2^* \end{pmatrix} - g_1 \begin{pmatrix} g_1^* & g_2^* \end{pmatrix} \right] \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix}$$

and

$$[(xx^* - gg^*)A]_{22} = \left[x_2 \begin{pmatrix} x_1^* & x_2^* \end{pmatrix} - g_2 \begin{pmatrix} g_1^* & g_2^* \end{pmatrix} \right] \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix}$$

Moreover, $A_{22}g_2 + A_{21}g_1 + a_2 = 0 \Longrightarrow \begin{pmatrix} g_1^* & g_2^* \end{pmatrix} \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} = -a_2^*$. And of course we know that $\begin{pmatrix} x_1^* & x_2^* \end{pmatrix} \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} = x_1^*A_{12} + x_2^*A_{22}$. Choose $y_2 = x_2 + A_{22}^{-1}(a_2 + A_{21}x_1)$ and we see that

$$[(xx^* - gg^*)A]_{12} = x_1y_2^*A_{22} - (x_1 - g_1)a_2^*$$

$$[(xx^* - gg^*)A]_{22} = y_2y_2^*A_{22} - A_{22}^{-1}(a_2 + A_{21}x_1)y_2^*A_{22} - (y_2 - g_2)a_2^* + A_{22}^{-1}(a_2 + A_{21}x_1)a_2^*$$

Then,

$$\begin{aligned}
[(G - gg^*)A]_{12} = \frac{1}{Z} \int & x_1 e^{-\frac{1}{2}x_1^*A_{11}x_1 - a_1^*x_1 - U(x_1)} \\
& \times \left(\int y_2^* e^{\frac{1}{2}(a_2 + A_{21}x_1)^* A_{22}^{-1}(a_2 + A_{21}x_1)} e^{-\frac{1}{2}y_2^*A_{22}y_2} \mathrm{d}y_2 \right) A_{22}\mathrm{d}x_1 \\
& - \frac{1}{Z} \int (x_1 - g_1)a_2^* e^{-\mathcal{H}(x)} \mathrm{d}x = 0
\end{aligned}$$

and

$$
\begin{aligned}
[(G-gg^*)A]_{22} &= \frac{1}{Z}\int e^{-\frac{1}{2}x_1^*A_{11}x_1-a_1^*x_1-U(x_1)} \\
&\times \left(y_2y_2^*e^{\frac{1}{2}(a_2+A_{21}x_1)^*A_{22}^{-1}(a_2+A_{21}x_1)}e^{-\frac{1}{2}y_2^*A_{22}y_2}\mathrm{d}y_2\right)A_{22}\mathrm{d}x_1 \\
&- \frac{1}{Z}\int A_{22}^{-1}(a_2+A_{21}x_1)e^{-\frac{1}{2}x_1^*A_{11}x_1-a_1^*x_1-U(x_1)} \\
&\times \left(\int y_2^*e^{\frac{1}{2}(a_2+A_{21}x_1)^*A_{22}^{-1}(a_2+A_{21}x_1)}e^{-\frac{1}{2}y_2^*A_{22}y_2}\mathrm{d}y_2\right)A_{22}\mathrm{d}x_1 \\
&- \frac{1}{Z}\int (y_2-g_2)a_2^*e^{-\mathcal{H}(x)}\mathrm{d}x_1\mathrm{d}y_2 \\
&+ \frac{1}{Z}\int A_{22}^{-1}(a_2+A_{21}x_1)a_2^*e^{-\mathcal{H}(x)}\mathrm{d}x_1\mathrm{d}y_2 \\
&= A_{22}^{-1}A_{22}+g_2a_2^*+A_{22}^{-1}a_2a_2^*+A_{22}^{-1}A_{21}g_1a_2^* \\
&= Id_q - A_{22}^{-1}(a_2+A_{21}g_1)a_2^*+A_{22}a_2a_2^*+A_{22}^{-1}A_{21}g_1a_2^* \\
&= Id_q
\end{aligned}
$$

which is equivalent to say that $\Sigma_{12}=0$ and $\Sigma_{22}=0$. Therefore, we reach our conclusion that $\Sigma_N = \begin{pmatrix}\Sigma_p & 0\\ 0 & 0\end{pmatrix}$. And the sparsity pattern that $\sigma_N = \begin{pmatrix}\sigma_p\\ 0\end{pmatrix}$ follows easily from the sparsity pattern of Σ_N and simple calculations.

Moreover, if we return to our statement of the transformation rule, we are confined to the case where the transformation $T \in GL_n(\mathbb{R})$ is general linear. In fact, other cases may occur. Consider an affine transform $\phi : x \mapsto Tx+b$, where T is invertible and $b \in \mathbb{R}^N$. And we want to explore any similar results to the "transformation rule" for the Luttinger Ward functional when the map ϕ is not necessarily linear.

Now,

$$
\begin{aligned}
\Phi[G,g,U\circ\phi] &= 2\mathcal{F}[G,g]-\mathrm{Tr}[\log(G-gg^*)]-N\log(2\pi e) \\
&= C-2\inf_{\rho\mathrm{d}x\in\mathcal{G}^{-1}(G)\cap\mathcal{P}^{-1}(g)}\left[\int(\log[(\det G-gg^*)^{1/2}\rho]+U\circ\rho)\rho\mathrm{d}x\right] \\
&= C-2|\det T|^{-1}\inf_{\rho\mathrm{d}x\in\mathcal{G}^{-1}(G)\cap\mathcal{P}^{-1}(g)}\left[\int(\log[(\det G-gg^*)^{1/2}\rho\circ\phi^{-1}]+U)\rho\circ\phi^{-1}\mathrm{d}x\right]
\end{aligned}
$$

Consider the change of variables

$$
\begin{aligned}
\{|\det T|^{-1}\cdot\rho\circ\phi^{-1}:\rho\mathrm{d}x\in\mathcal{G}^{-1}(G)\cap\mathcal{P}^{-1}(g)\} &= \{\rho:|\det T|\cdot\rho\circ\phi\in\mathcal{G}^{-1}(G)\cap\mathcal{P}^{-1}(g)\} \\
&= \{\rho:\rho\mathrm{d}x\in\mathcal{G}^{-1}(TGT^*+Tgb^*+bg^*T^*+bb^*)\cap\mathcal{P}^{-1}(Tg+b)\}
\end{aligned}
$$

because $|\det T|\cdot\rho\circ\phi \in \mathcal{G}^{-1}(G)\cap\mathcal{P}^{-1}(g) \iff \int xx^*\rho(Tx+b)\mathrm{d}x = G\cdot|\det T|^{-1}$ and $\int x\rho(Tx+b)\mathrm{d}x = g\cdot|\det T|^{-1} \iff \int(yy^*-yb^*-by^*)\rho\mathrm{d}y = TGT^*-bb^*$ and $\int(y-b)\rho\mathrm{d}y = Tg \iff \int yy^*\rho\mathrm{d}y = TGT^*+Tgb^*+bg^*T^*+bb^*$ and $\int y\rho\mathrm{d}y = Tg+b$, which verifies the change of variables.

For simplicity, we denote the condition that $\rho\mathrm{d}x \in \mathcal{G}^{-1}(TGT^*+Tgb^*+bg^*T^*+bb^*)\cap\mathcal{P}^{-1}(Tg+b)$ as $\rho\mathrm{d}x\in\mathbb{P}$. Then,

$$
\Phi[G,g,U\circ\phi] = C-2\inf_{\rho\mathrm{d}x\in\mathbb{P}}\left[\int(\log\left[(\det G-gg^*)^{1/2}|\det T|\rho\right]+U)\rho\mathrm{d}x\right]
$$

However,

$$
|\det T|\big(\det G-gg^*\big) = \det\Big(TGT^*+Tgb^*+bg^*T^*+bb^*-(Tg+b)(Tg+b)^*\Big)
$$

Therefore, we reach our conclusion that

$$\Phi[G, g, U \circ \phi] = \Phi[TGT^* + Tgb^* + bg^*T^* + bb^*, Tg + b, U]$$

where $x \xrightarrow{\phi} Tx + b$ is our affine transform.

In the old setting where $\mathcal{H}(x) = \frac{1}{2}x^*Ax + U(x)$, we have established the Legendre correspondence relations $\nabla\mathcal{F}[G] = A[G]$, $\nabla\Omega[A] = G[A]$ and Φ-derivative $\Sigma[G] = \frac{1}{2}\nabla_G\Phi[G, U]$. When we add a linear term to our new Hamiltonian, it becomes $\mathcal{H}(x) = \frac{1}{2}x^*Ax + a^*x + U(x)$.

In this new setting, we would like to know whether there exists any similar relations among these physical quantities. Now, the partition function $Z = \int e^{-\mathcal{H}(x)}\mathrm{d}x$. And the free energy

$$\Omega[A, a] = -\log Z = -\int \exp\left\{-\frac{1}{2}x^*Ax - a^*x - U(x)\right\}\mathrm{d}x$$

By matrix differentiation, we see

$$\nabla_A\Omega[A, a] = \frac{1}{Z}\int xx^*e^{-\mathcal{H}(x)}\mathrm{d}x = G$$

and

$$\nabla_a\Omega[A, a] = \frac{1}{Z}\int xe^{-\mathcal{H}(x)}\mathrm{d}x = g$$

And given the Legendre dual

$$\mathcal{F}[G, g] = \sup_{\mu\in\mathcal{G}^{-1}(G)\cap\mathcal{P}^{-1}(g)}\left[H(\mu) - \int U\mathrm{d}\mu\right]$$

via a delicate analysis of concave functions, we find

$$\nabla_G\mathcal{F}[G, g] = A, \quad \text{and} \quad \nabla_g\mathcal{F}[G, g] = a$$

In this regard we have shown the mapping $(A, a) \mapsto (\nabla_A\Omega, \nabla_a\Omega)$ with its inverse $(G, g) \mapsto (\nabla_G\mathcal{F}, \nabla_g\mathcal{F})$.

Moreover, we already know the Luttinger Ward functional

$$\Phi[G, g, U] = 2\mathcal{F}[G, g] - \mathrm{Tr}[\log(G - gg^*)] - N\log(2\pi e)$$

Then,

$$\begin{aligned}\frac{1}{2}\nabla_G\Phi &= \nabla_G\mathcal{F}[G, g] - \frac{1}{2}\nabla_G\,\mathrm{Tr}[\log(G - gg^*)]\\ &= A - (G - gg^*)^{-1}\end{aligned}$$

On the other hand,

$$\begin{aligned}\frac{1}{2}\nabla_g\Phi &= \nabla_g\mathcal{F}[G, g] - \frac{1}{2}\nabla_g\,\mathrm{Tr}[\log(G - gg^*)]\\ &= a - (G - gg^*)^{-1}\cdot\frac{1}{2}\cdot(-2g)\\ &= a + (G - gg^*)^{-1}g\end{aligned}$$

where we use the result that the differential of the map $g \mapsto gg^*$ is the linear map $g \mapsto g$. Hence, the Φ-derivable self energies

$$\frac{1}{2}\nabla_G\Phi = \Sigma, \quad \text{and} \quad \frac{1}{2}\nabla_g\Phi = \sigma$$

Now we discuss the DMFT algorithm in this setting. Consider $M = RL$, and the interaction $U_c : x_c \in \mathbb{R}^L \mapsto U_c(x_c)$, $c = 1, \cdots, R$ satisfying the weak growth condition. We define the Gibbs measure

$$\mathrm{d}\mu(x) = e^{-\frac{1}{2}x^* Ax - a^* x} \prod_{1\le c\le R} e^{-U_c(x_c)} \mathrm{d}x_c$$

We want to compute the exact hybridization $\Delta \in \mathbb{R}^{M\times M}$ and $\delta \in \mathbb{R}^M$ such that the other measure

$$\bigotimes_{1\le c\le R} \mathrm{d}\mu_c(x_c) = \prod_{1\le c\le R} e^{-\frac{1}{2}x_c^*(A_c+\Delta_c)x_c-(a_c+\delta_c)^* x_c - U_c(x_c)} \mathrm{d}x_c$$

has the same diagonal (local) Green's functions (second moments) $G_c \in \mathbb{R}^{L\times L}$ and first moments $g_c \in \mathbb{R}^L$.

We are interested in the case where the interactions are extremized, forming into an Ising model. But of course, there is now an extre linear term in the Hamiltonian. Hence, from the given global Gibbs measure

$$\mathrm{d}\mu(x) = e^{-\frac{1}{2}x^* Ax - a^* x} \prod_{c=1}^{R} \sum_{\sigma\in\{-1,1\}^L} \mathrm{d}\delta(x_c - \sigma)$$

we want to compute the (local) exact hybridization $\Delta_c \in \mathbb{R}^{L\times L}$ and $\delta_c \in \mathbb{R}^L$ such that the product measure $\otimes_{c=1}^R \mathrm{d}\mu_c(x_c)$ has the same second moments $G_c \in \mathbb{R}^{L\times L}$ and first moments $g_c \in \mathbb{R}^L$ as the original measure, where

$$\mathrm{d}\mu_c(x_c)) = e^{-\frac{1}{2}x_c^*(A_c+\Delta_c)x_c-(a_c+\sigma_c)*x_c-U_c(x_c)} \sum_{\sigma\in\{-1,1\}^L} \delta(x_c - \sigma)$$

Hence, given the explicit solutions $\{(\Delta_c, \delta_c), 1 \le c \le R\}$, we have

$$G_c = \langle x_c x_c^* \rangle_{\mu_c} = \sum_{\sigma\in\{-1,1\}^L} \sigma\sigma^* e^{-\frac{1}{2}\sigma^*(A_c+\Delta_c)\sigma-(a_c+\delta_c)^*\sigma} \Big/ \sum_{\sigma} e^{-\frac{1}{2}\sigma^*(A_c+\Delta_c)\sigma-(a_c+\delta_c)^*\sigma}$$

and

$$g_c = \langle x_c \rangle_{\mu_c} = \sum_{\sigma\in\{-1,1\}^L} \sigma e^{-\frac{1}{2}\sigma^*(A_c+\Delta_c)\sigma-(a_c+\delta_c)^*\sigma} \Big/ \sum_{\sigma} e^{-\frac{1}{2}\sigma^*(A_c+\Delta_c)\sigma-(a_c+\delta_c)^*\sigma}$$

Given the above discussions, we come to the DMFT algorithm to compute the exact hybridization $\{(\Delta_c, \delta_c), 1 \le c \le R\}$ and hopefully we could approximate the product measure $\otimes_{c=1}^R \mathrm{d}\mu_c(x_c)$.

Initially, we choose $\Delta_c^{(0)} = 0$, $\delta_c^{(0)}$. Then,

$$\mathrm{d}\mu_c^{(0)}(x_c) = e^{-\frac{1}{2}x_c^* A_c x_c - a_c^* x_c} \sum_{\sigma\in\{-1,1\}^L} \mathrm{d}\delta(x_c - \sigma)$$

And we compute the (local) partition function

$$Z_c^{(0)} = \int \mathrm{d}\mu_c^{(0)} = \sum_{\sigma\in\{-1,1\}^L} e^{-\frac{1}{2}\sigma^* A_c \sigma - a_c^*\sigma}$$

And the (local) 2^{nd} and 1^{st} moments

$$G_c^{(0)} = \langle x_c x_c^* \rangle_{\mu_c^{(0)}}, \quad \text{and} \quad g_c^{(0)} = \langle x_c \rangle_{\mu_c^{(0)}}$$

Remember that we have the global relations

$$A - (G - gg^*)^{-1} = \Sigma, \quad \text{and} \quad a + (G - gg^*)^{-1} g = \sigma$$

Then we define

$$\Sigma_c^{(0)} = A_c + \Delta_c^{(0)} - (G_c^{(0)} - g_c^{(0)} g_c^{(0)*})^{-1}$$

and

$$\sigma_c^{(0)} = a_c + \delta_c^{(0)} + (G_c^{(0)} - g_c^{(0)} g_c^{(0)*})^{-1} g_c^{(0)}$$

Then, via the direct sum, we define

$$\Sigma^{(0)} = \bigoplus_{1 \le c \le R} \Sigma_c^{(0)}, \quad \text{and} \quad \sigma^{(0)} = \bigoplus_{1 \le c \le R} \sigma_c^{(0)}$$

Hence we wet the iterative (global) 2^{nd} and 1^{st} moments

$$G^{(0)} = (A + \Lambda^{(0)} - \Sigma^{(0)})^{-1} + (\oplus_{c=1}^R g_c^{(0)})(\oplus_{c=1}^R g_c^{(0)*})$$

and

$$g^{(0)} = \big((\oplus_{c=1}^R G_c^{(0)}) - (\oplus_{c=1}^R g_c^{(0)})(\oplus_{c=1}^R g_c^{(0)*})\big)(\sigma^{(0)} - a)$$

Let $\pi_c : \mathbb{R}^M \to \mathbb{R}^L$ be the canonical projection to the c^{th} cluster, we define the iteration

$$\Delta_c^{(1)} = \Sigma_c^{(0)} - A_c + (\pi_c G^{(0)} \pi_c^* - \pi_c g^{(0)} g^{(0)*} \pi_c^*)^{-1}$$

and

$$\delta_c^{(1)} = \sigma_c^{(0)} - a_c - (\pi_c G^{(0)} \pi_c^* - \pi_c g^{(0)} g^{(0)*} \pi_c^*)^{-1} (\pi_c g^{(0)})$$

Hence the iteration continues and $\forall n \in \mathbb{N}$,

$$G_c^{(n)} = \langle x_c x_c^* \rangle_{\mu_c^n} = \sum_{\sigma \in \{-1,1\}^L} \sigma\sigma^* e^{-\frac{1}{2}\sigma^*(A_c + \Delta_c^{(n)})\sigma - (a_c + \delta_c^{(n)})^* \sigma} \Bigg/ \sum_{\sigma \in \{-1,1\}^L} e^{-\frac{1}{2}\sigma^*(A_c + \Delta_c^{(n)})\sigma - (a_c + \delta_c^{(n)})^* \sigma}$$

and

$$g_c^{(n)} = \langle x_c \rangle_{\mu_c^n} = \sum_{\sigma \in \{-1,1\}^L} \sigma e^{-\frac{1}{2}\sigma^*(A_c + \Delta_c^{(n)})\sigma - (a_c + \delta_c^{(n)})^* \sigma} \Bigg/ \sum_{\sigma \in \{-1,1\}^L} e^{-\frac{1}{2}\sigma^*(A_c + \Delta_c^{(n)})\sigma - (a_c + \delta_c^{(n)})^* \sigma}$$

And the n^{th} (local) self-energy,

$$\Sigma_c^{(n)} = A_c + \Delta_c^{(n)} - (G_c^{(n)} - g_c^{(n)} g_c^{(n)*})^{-1}$$

and

$$\sigma_c^{(n)} = a_c + \delta_c^{(n)} + (G_c^{(n)} - g_c^{(n)} g_c^{(n)*})^{-1} g_c^{(n)}$$

And the n^{th} (global) self-energy comes from direct sums

$$\Sigma^{(n)} = \bigoplus_{1 \le c \le R} \Sigma_c^{(n)}, \quad \text{and} \quad \sigma^{(n)} = \bigoplus_{1 \le c \le R} \sigma_c^{(n)}$$

And the 2^{nd} and 1^{st} moments

$$G^{(n)} = (A + \Lambda^{(n)} - \Sigma^{(n)})^{-1} + (\oplus_{c=1}^R g_c^{(n)})(\oplus_{c=1}^R g_c^{(n)*})$$

and

$$g^{(n)} = \big((\oplus_{c=1}^R G_c^{(n)}) - (\oplus_{c=1}^R g_c^{(n)})(\oplus_{c=1}^R g_c^{(n)*})\big)(\sigma^{(n)} - a)$$

And the iterated exact hybridization,

$$\Delta_c^{(n+1)} = \Sigma_c^{(n)} - A_c + (\pi_c G^{(n)} \pi_c^* - \pi_c g^{(n)} g^{(n)*} \pi_c^*)^{-1}$$

and

$$\delta_c^{(n+1)} = \sigma_c^{(n)} - a_c - (\pi_c G^{(n)} \pi_c^* - \pi_c g^{(n)} g^{(n)*} \pi_c^*)^{-1} (\pi_c g^{(n)})$$

where $\Lambda^{(n)} \in \mathbb{R}^{M \times M}$, $\Lambda^{(n)} = \mathrm{diag}(\lambda^{(n)})$ are similarly defined as $\Lambda^{(0)}$ to ensure that $\mathrm{diag}(G^{(n)}) = Id_M$. Notice that we could use Metropolis algorithm to solve explicitly for $\Lambda^{(n)}$ once we are fully convinced that a unique $\Lambda^{(n)} = \mathrm{diag}(\lambda^{(n)})$ exists.

6 One-Site Clusters

Consider the Ising model [1] with 1-site clusters. This model may not seem to be very good approximation, in the sense that all quadratic part of the hybridization $\{(\Delta_c, \delta_c), 1 \le c \le R\}$ vanishes. So there is essentially one variable. Other very important phenomena and formulations are also presented in [5, 8, 9]. These references mark essential progress in Statistical Mechanics.

In this setting, $L = 1$, and $M = R$, $1 \le c \le M$. Choose $\Delta_c^{(0)} = 0$, $\delta_c^{(0)} = 0$, and

$$\mathrm{d}\mu_c^{(0)}(x_c) = \sum_{\sigma \in \{-1,1\}^L} e^{-\frac{1}{2} A_c x_c^2 - a_c x_c} \, \mathrm{d}\delta(x_c \pm 1)$$

Then the initial partition function

$$Z_c^{(0)} = \int \mathrm{d}\mu_c^{(0)} = e^{-\frac{1}{2} A_c} (e^{a_c} + e^{-a_c}) = 2e^{-\frac{1}{2} A_c} \cosh a_c$$

And the (local) 2^n and 1^{st} moments

$$G_c^{(0)} = \langle x_c^2 \rangle_{\mu_c^{(0)}} = 1$$

and

$$g_c^{(0)} = \langle x_c \rangle_{\mu_c^{(0)}} = 2e^{-\frac{1}{2} A_c} \cdot \frac{e^{-a_c} - e^{a_c}}{Z_c^{(0)}} = -\tanh a_c$$

And then the initial self energy

$$\Sigma_c^{(0)} = A_c - (1 - \tanh^2 a_c)^{-1} = A_c - \cosh^2 a_c$$

and

$$\sigma_c^{(0)} = a_c - (1 - \tanh^2 a_c)^{-1} \tanh a_c = a_c - \cosh a_c \sinh a_c$$

And via direct sums,

$$\Sigma^{(0)} = \bigoplus_{1 \le c \le M} \Sigma_c^{(0)} = A_c \cdot Id_M - \mathrm{diag}(\cosh^2 a_c, 1 \le c \le M)$$

and

$$\sigma^{(0)} = \bigoplus_{1 \le c \le M} \sigma_c^{(0)} = a - (\cosh a_c \sinh a_c, \, 1 \le c \le M)^T$$

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