A classical statistical mechanics approach to understanding Green's function methods and the Luttinger-Ward formalism

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(Joint work with Lin Lin)

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Introduction

- Caution: this is a lateral move from quantum physics/chemistry
- Nonetheless, can interpret: Green's functions, self-energy, Luttinger-Ward functional, bare diagrams, bold diagrams, bold screened diagrams, Hartree-Fock, GW, Hedin's equations, screening (or lack thereof) of Coulomb interaction, impurity problems, DMFT, DMFT+ ___ , etc.
- Testing ground for numerical evaluation of Green's function methods
- Necessary waypoint for mathematical understanding
- Direct application to statistical-mechanical systems including ϕ^4 (and nonlocal generalization), Landau-Ginzburg-Wilson, etc.
- Connection with classical spin systems
- See Lin Lin, M.L. PNAS (2018), upcoming longer math paper

Gibbs model

- Fix *interaction* $U : \mathbb{R}^n \to \mathbb{R}$, define the partition function $Z : \mathcal{S}^n \to \mathbb{R}$ as a function on the set of symmetric matrices:

$$Z[A] = \int e^{-\frac{1}{2}x^T A x - U(x)}\, dx$$

- Then define the Gibbs free energy $\Omega : \mathcal{S}^n \to \mathbb{R}$

$$\Omega[A] = -\log Z[A].$$

- Define the two-point correlator (Green's function)

$$G[A] := \nabla_A \Omega[A] = \frac{1}{Z[A]} \int x x^T\, e^{-\frac{1}{2}x^T A x - U(x)}\, dx.$$

- In noninteracting case ($U \equiv 0$), $G = G_0 = A^{-1}$
- Appropriate analog of Coulomb interaction is

$$U(x) = \frac{1}{8} \sum_{ij} v_{ij} x_i^2 x_j^2$$

  where v is positive definite

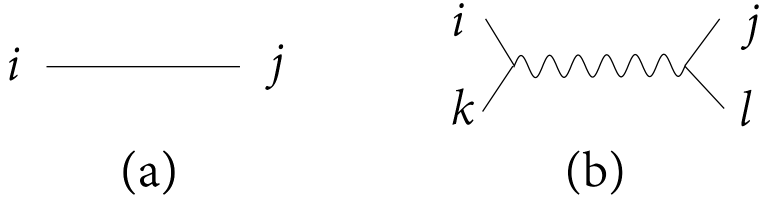
Perturbation theory and (bare) Feynman diagrams

- Idea is that, formally, e.g.,

$$\begin{aligned} Z[A] &= \int e^{-U(x)} e^{-\frac{1}{2}x^T A x}\, dx \\ &= \sum_{k=0}^{\infty} \frac{1}{n!} \int [-U(x)]^n e^{-\frac{1}{2}x^T A x}\, dx. \end{aligned}$$

- Using Wick/Isserlis theorem, can compute formal power series expansion in terms of G_0 and v
- Caution: only get asymptotic series!
- Power series can be organized graphically via Feynman diagrams

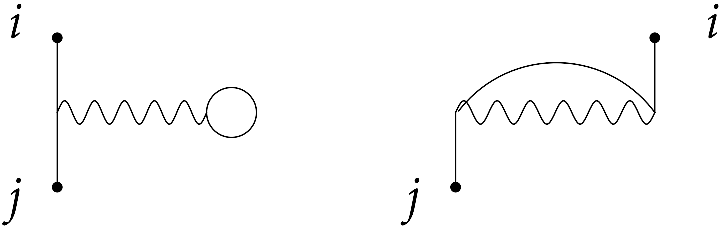
Diagrammatic building blocks



(a): $(G_0)_{ij}$

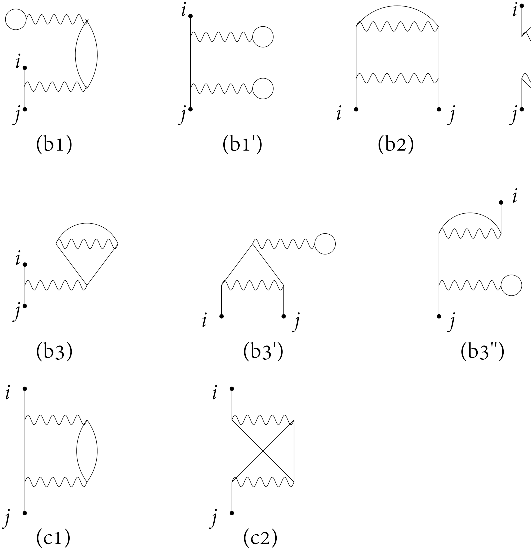
(b): $-v_{ij}\delta_{ik}\delta_{jl}$

Feynman diagrams for G (first order)



(a) (b)

Feynman diagrams for G (second order)



The self-energy

- Want to organize the expansion
- Σ "$=$" sum of one-particle irreducible (amputated) diagrams
- Designed to satisfy

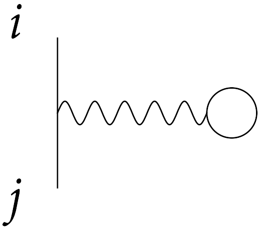
$$G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \dots$$

- Could also have defined via Dyson equation:

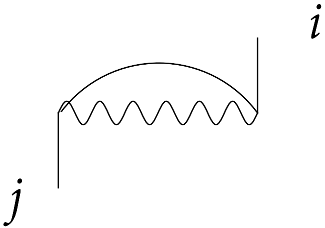
$$G^{-1} = G_0^{-1} - \Sigma$$

- This can be written $G = G_0 + G_0 \Sigma G$

Self-energy diagrams (first order)

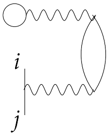


(a)

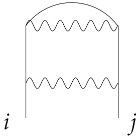


(b)

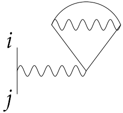
Self-energy diagrams (second order)



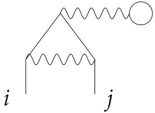
(b1)



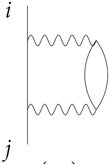
(b2)



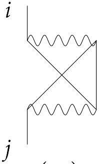
(b3)



(b3')

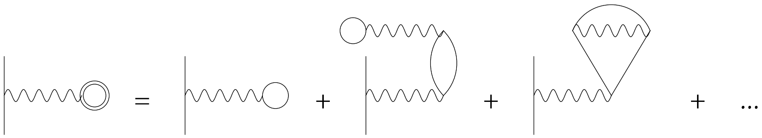


(c1)



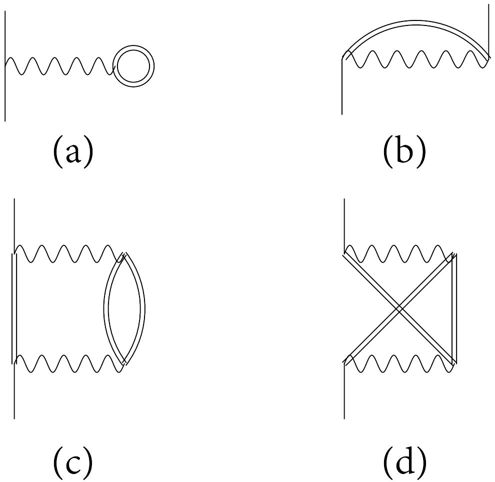
(c2)

Bold self-energy diagrams



Double line $= G$ (dressed/renormalized propagator)

Self-energy diagrams (first and second order)



Bold diagrams

- $\Sigma = \Sigma[G]$?
- Use in combination with Dyson equation $G^{-1} = A - \Sigma[G]$ to derive self-consistent Green's function methods
- In fact, we'll see that $\Sigma[G] = \nabla_G \Phi[G]$; an ansatz for Φ yields a so-called Φ-derivable Green's function method
- Derivation involved an infinite partial resummation of a (divergent!) series. How to interpret rigorously?

Back to Earth

- Recall that $\Omega : \mathcal{S}^n \to \mathbb{R}$ is the log-partition function and $G[A] = \nabla_A \Omega[A]$
- Ω is strictly concave and smooth, so expect that G is a bijection onto its range
- Want to examine concave dual

The dual side

- Define concave dual
$$\mathcal{F}[G] := \Omega^*[G] = \inf_{A \in \mathcal{S}^n} \left(\frac{1}{2} \mathrm{Tr}[AG] - \Omega[A] \right)$$
- Can show
$$\mathcal{F}[G] = \sup_{\mu \mapsto G} \left(S(\mu) - \int U \, d\mu \right)$$
via contraction of classical Gibbs variational principle (cf. Levy-Lieb)
- $\mathrm{dom}(\mathcal{F}) = \mathcal{S}^n_{++}$
- Duality says $G = G[A]$ is a bijection $\mathcal{S}^n \to \mathcal{S}^n_{++}$ with inverse given by $A[G] = \nabla_G \mathcal{F}[G]$

The Luttinger-Ward functional

- Define

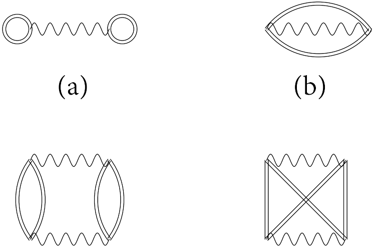
$$\Phi[G] := 2\mathcal{F}[G] - \mathrm{Tr}\log[G] - n\log(2\pi e)$$

- Defined so that $\Phi \equiv 0$ in noninteracting case $U \equiv 0$
- **Theorem**: Φ extends continuously up to the boundary of $\mathcal{S}^n_{++}$ for general U (of sufficient growth); behavior on boundary described in terms of lower-dimensional LW functionals
- Define self-energy $\Sigma[G] := \nabla_G \Phi[G]$
- Stationarity implies Dyson equation

$$G^{-1} = A - \Sigma[G] = G_0^{-1} - \Sigma[G]$$

Bold diagrams revisited

- Consider dependence of Φ, Σ on interaction via $\Phi[G, U]$, $\Sigma[G, U]$
- **Theorem**: bold self-energy diagrams are an asymptotic series at $\varepsilon = 0$ for $\Sigma[G, \varepsilon U]$; moreover, k-th coefficient in asymptotic series for LW functional is given by $\Phi^{(k)} = \frac{1}{2k}\mathrm{Tr}[G\Sigma^{(k)}]$
- LW diagrams:



(a) (b) (c) (d)

What have we done?

- Analytically, we defined concave dual of free energy, subtracted divergent part (motivated by noninteracting picture)
- Diagrammatically, this corresponded to the renormalization of bare to bold diagrams
- Huh!

Large-interaction limit

- Consider ‘Coulomb’ interaction with matrix λv as $\lambda \to +\infty$
- Can we understand LW theory in this limit? (Via scaling relation for LW, equivalent to looking at limit of large G)
- Partial answer: for fixed G in a certain set (large but not everything)

$$\begin{aligned}
&\mathcal{F}_\lambda[G] + \frac{n}{2}\log\left(\frac{\lambda}{2\pi}\right) + \frac{\lambda}{8}\sum_{ij} v_{ij}G_{ii}G_{jj} \\
= \quad &\widehat{\mathcal{F}}[g^{-1}Gg] - \frac{1}{2}\mathrm{Tr}\log v - \frac{1}{2}\sum_{i=1}^{n}\log G_{ii} + O(\lambda^{-1}),
\end{aligned}$$

where $g = \mathrm{diag}(\sqrt{G_{11}}, \ldots, \sqrt{G_{nn}})$ and $\widehat{\mathcal{F}}$ is a functional derived from Legendre duality for spin systems

Other developments and directions

- Further analytical and numerical study of GW (and extensions)
- Impurity problems (U depends only on a subset of the variables) and DMFT
- Try to resolve mysteries in quantum many-body case, see Kozik et al., PRL (2015), Gunnarsson et al., PRL (2017)
- In quantum many-body setting, Green's functions are frequency-dependent! What is the correct domain? PRPRP?