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Variational structure of Luttinger–Ward formalism and bold diagrammatic expansion for Euclidean lattice field theory

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The Luttinger–Ward functional was proposed more than five decades ago and has been used to formally justify most practically used Green’s function methods for quantum many-body systems. Nonetheless, the very existence of the Luttinger–Ward functional has been challenged by recent theoretical and numerical evidence. We provide a rigorously justified Luttinger–Ward formalism, in the context of Euclidean lattice field theory. Using the Luttinger–Ward functional, the free energy can be variationally minimized with respect to Green’s functions in its domain. We then derive the widely used bold diagrammatic expansion rigorously, without relying on formal arguments such as partial resummation of bare diagrams to infinite order.

many-body perturbation theory | Feynman diagrams | lattice field theory | Luttinger–Ward formalism | Green’s function

The Luttinger–Ward (LW) formalism (1) is an important component of Green’s function theories in quantum many-body physics. The LW functional $\Phi[G]$ provides the formal foundation for bold diagrammatic perturbation theory to all orders and is used to formally derive widely used numerical schemes such as the self-consistent Hartree–Fock approximation, the GW approximation (2), the dynamical mean-field theory (DMFT) (3, 4), and a number of its recent extensions such as the DMFT+GW method (5) and the dynamical cluster approximation (6). Nonetheless, the very existence of the LW functional is currently under debate, with theoretical and numerical evidence favoring the contrary in the past few years for fermionic systems (7–10). Such failure has profound theoretical and practical implications. It suggests that many practically used Green’s functions for computing static or dynamic properties might fail in unpredictable ways. In particular, even in the perturbative regime where bare diagrams converge, the bold diagrams may fail to converge or converge to the wrong quantity (7).

In this work, we provide a rigorously justified LW formalism, in the context of the Euclidean lattice field theory [such as the φ^4 theory (11, 12)]. Due to an exact correspondence between the Feynman diagrammatic expansion of lattice field theory and that of quantum many-body physics (11, 13), Euclidean lattice field theory retains the valuable structural information of diagrammatic expansions. Meanwhile, it avoids a key theoretical challenge of the fermionic setup, in the sense that the Green’s function in the Euclidean lattice field theory, defined as a two-point correlator function, has a clearly defined domain, namely the set of positive definite matrices. Hence this work represents a key step toward understanding and potentially remedying the LW formalism and Green’s function methods for fermionic systems. Our theory also proves the widely used bold diagrammatic expansion, interpreted as an asymptotic series for approximating the LW functional. Independently, our adaptation of the LW formalism to a different setting may provide unique insight into the study of Euclidean field theories.

For a general interaction form (not necessarily the quartic interaction), we prove using Legendre duality that there

exists a universal functional of the Green’s function, denoted $\mathcal{F}[G]$, which is defined via a constrained minimization problem similar in spirit to that of the Levy–Lieb construction in density functional theory (14, 15) at zero temperature and the Mermin functional (16) at finite temperature and further the “density matrix functional theory” developed in refs. 17–19. We identify a natural one-to-one correspondence between the interacting Green’s function G and the inverse G_0^{-1} of the noninteracting Green’s function. The LW functional $\Phi[G]$ is rigorously defined by subtracting a logarithmically divergent component from $\mathcal{F}[G]$. The functional derivative of the LW functional defines the self-energy and is also universal. The free energy can be expressed variationally as a minimum over all physical Green’s functions, and the self-consistent solution of the Dyson equation yields its global and unique minimizer. Finally, using the LW formalism for quartic interactions, we rigorously recover the form of the bold diagrammatic expansion appearing in the quantum many-body setting, without any reference to the noninteracting Green’s function G_0 . This work gives our main results and outlines of the proofs.

After proper discretization, a Euclidean lattice field theory can be described by the partition function

$$Z = \int_{\mathbb{R}^n} e^{-\frac{1}{2}x^T Ax - U(x)} dx. \quad [1]$$

For instance, the partition function of a scalar φ^4 theory in a d -dimensional space is

Significance

Many-body perturbation theory is one of the pillars of quantum many-body physics and has been used extensively to predict ground-state and excited-state electronic properties of real materials in the past few decades. Nonetheless, few practically used methods in many-body perturbation theory have been justified on a rigorous basis. We present a variational formalism that can be used for the rigorous study of a number of many-body perturbation methods in Euclidean lattice field theory. In particular, this perspective allows us to justify the widely used bold Feynman diagrammatic expansion, without relying on formal arguments such as partial resummation of Feynman diagrams to infinite order.

Author contributions: L.L. and M.L. designed research, performed research, and wrote the paper.

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$$Z = \int \mathcal{D}\varphi(\mathbf{r}) e^{-\int_{\mathbb{R}^d} \frac{1}{2} |\nabla\varphi(\mathbf{r})|^2 + u\varphi^2(\mathbf{r}) + v\varphi^4(\mathbf{r}) \, d\mathbf{r}}. \quad [2]$$

After discretizing the field $\varphi(\mathbf{r})$ on a lattice of size n with components denoted by $\{x_i\}_{i=1}^n$, we can rewrite the quadratic part in Eq. 2 by a quadratic form given by a symmetric matrix A and the quartic part by a polynomial $U(x)$ as in Eq. 1. Here A can be associated with the noninteracting Hamiltonian in quantum many-body physics and U with the interaction term. The form in Eq. 1 is very general and can represent interaction terms that are quartic, beyond quartic, or even nonpolynomial in classical and quantum statistical mechanics (e.g., refs. 11, 20, and 21). For the integral to be well defined, we assume that $U(x)$ goes to infinity faster than any quadratic function of x . More precisely, we assume that for any $\alpha \in \mathbb{R}$, there exists a constant $b \in \mathbb{R}$ such that $U(x) + b \geq \alpha \|x\|^2$ for all $x \in \mathbb{R}^n$. This is referred to as the strong growth condition for U . The growth condition can be weakened so that our theory is applicable to a larger class of interactions, but we do not discuss such technical details in this paper. For simplicity we restrict our attention to real matrices, although analogous results can be obtained in the complex Hermitian case.

Let S^n , S_+^n , and S_{++}^n denote, respectively, the sets of symmetric, symmetric positive semidefinite, and symmetric positive definite real $n \times n$ matrices, so $S_{++}^n \subset S_+^n \subset S^n$. Then the partition function Z in Eq. 1 can be viewed as a functional of $A \in S^n$ denoted by $Z[A]$. The Gibbs free energy is defined as $\Omega[A] := -\log Z[A]$, and $\Omega[A]$ is strictly concave and C^∞ smooth on S^n .

The derivative of Ω with respect to A_{ij} defines the two-point correlator or the Green's function

$$G_{ij} := \nabla_{ij} \Omega[A] = \frac{1}{Z[A]} \int x_i x_j e^{-\frac{1}{2} x^T A x - U(x)} \, dx. \quad [3]$$

The matrix $G \in S^n$ is the two-point correlator with respect to the probability distribution $\rho(x) = e^{-\frac{1}{2} x^T A x - U(x)} / Z[A]$, and hence $G \in S_{++}^n$. G is called the interacting Green's function, and if we set $U(x) \equiv 0$, we obtain the noninteracting Green's function $G_0 = A^{-1}$. However, the noninteracting Green's function G_0 is well defined only for $A \in S_{++}^n$, while the interacting Green's function G is well defined for any $A \in S^n$ owing to the growth property of the interaction term $U(x)$.

Let \mathcal{M} be the space of probability density functions on \mathbb{R}^n with moments up to second order; i.e., let

$$\mathcal{M} = \left\{ \rho \in L^1(\mathbb{R}^n, (1 + |x|^2) \, dx) : \rho \geq 0, \int \rho(x) \, dx = 1 \right\}.$$

Define $\mathcal{G} : \mathcal{M} \rightarrow S_{++}^n$ by $\mathcal{G}(\rho) = \int x x^T \rho \, dx$, which maps a probability density to a Green's function in S_{++}^n . On the other hand, for any $G \in S_{++}^n$, it is clear that the inverse mapping $\mathcal{G}^{-1}(G)$ is a nonempty set through the construction of a Gaussian distribution. For a general interaction $U : \mathbb{R}^n \rightarrow \mathbb{R}$ satisfying the strong growth condition, our main results are given in *Theorems 1 and 2*.

Theorem 1 (Variational Structure). *The Gibbs free energy $\Omega : S^n \rightarrow \mathbb{R}$ can be expressed variationally via*

$$\Omega[A] = \inf_{G \in S_{++}^n} \left(\frac{1}{2} \text{Tr}[AG] - \mathcal{F}[G] \right), \quad [4]$$

where $\mathcal{F} : S_{++}^n \rightarrow \mathbb{R}$, defined as

$$\mathcal{F}[G] := \sup_{\rho \in \mathcal{G}^{-1}(G)} \left[S(\rho) - \int U \rho \, dx \right], \quad [5]$$

is the Legendre dual of $\Omega[A]$ with respect to the inner product $\langle A, G \rangle = \frac{1}{2} \text{Tr}[AG]$. Here $S : \mathcal{M} \rightarrow \mathbb{R}$ is the entropy and is defined

as $S(\rho) = -\int \rho \log \rho \, dx$. The mapping $G[A] := \nabla \Omega[A]$ is a bijection $S^n \rightarrow S_{++}^n$, with the inverse given by $A[G] := \nabla \mathcal{F}[G]$.

Note that \mathcal{F} depends only on G and, implicitly, on the interaction U , but it is independent of the noninteracting term A . In this sense, \mathcal{F} is a universal functional of the Green's function G .

The last statement of *Theorem 1* suggests that $\nabla \mathcal{F}$ (hence also \mathcal{F}) should approach infinity as G approaches the boundary of S_{++}^n . Remarkably, we can explicitly separate the part that accounts for the blowup of \mathcal{F} at the boundary. Consider the case in which $U \equiv 0$ and $\mathcal{F}[G] = \sup_{\rho \in \mathcal{G}^{-1}(G)} S(\rho)$. The maximum is attained by the probability density corresponding to the Gaussian distribution $\mathcal{N}(0, G)$, whose entropy is $\frac{1}{2} \log \det(2\pi e G)$. Hence

$$\mathcal{F}[G] = \frac{1}{2} \log((2\pi e)^n \det G) = \frac{1}{2} \text{Tr}[\log(G)] + \frac{n}{2} \log(2\pi e), \quad [6]$$

which diverges logarithmically as G approaches the boundary of S_{++}^n . Subtracting away this singular part, we define the LW functional as

$$\Phi[G] := 2\mathcal{F}[G] - \text{Tr}[\log(G)] - \Phi_0, \quad \Phi_0 = n \log(2\pi e). \quad [7]$$

Theorem 2 (LW Functional). *The LW functional in Eq. 7 is universal, satisfies $\Phi[G] \equiv 0$ for noninteracting systems, and extends continuously up to the boundary of S_{++}^n . The self-energy functional is defined as $\Sigma[G] = \nabla \Phi[G]$ and is also universal. The solution of the Dyson equation*

$$G^{-1} = A - \Sigma[G] \quad [8]$$

in S_{++}^n is the unique minimizer of the free energy in Eq. 4.

According to the preceding discussion, for $A \in S_{++}^n$, we have $G_0 = A^{-1}$, and the Dyson equation Eq. 8 can be written equivalently as

$$G = G_0 + G_0 \Sigma[G] G. \quad [9]$$

This is the common starting point for deriving the Feynman diagram expansion (11, 13) with propagator G_0 , i.e., the “thin-line” (or “bare”) diagrammatic expansion. In our setting, this expansion is meaningless when $A \notin S_{++}^n$, since the corresponding partition function Eq. 1 diverges in noninteracting limit. On the other hand, the Dyson equation in the form of Eq. 8 is more general and is valid for any $A \in S^n$.

When the self-energy functional $\Sigma[G]$ is known, Eq. 8 can be solved to obtain G . On the other hand, Eq. 8 can also be used in the reverse direction to compute Σ once A and an approximation to G are available. This is the approach taken in DMFT (3), which approximates Σ by solving a number of impurity problems on local domains. This second use of the Dyson equation seems to suggest that Σ depends on both G and A , although we have claimed it to be a universal functional of G ! However, the one-to-one mapping between A and G furnished by *Theorem 1* resolves this paradox, and $\Sigma[G]$ is indeed well defined for the Euclidean lattice field theory. A similar correspondence for many-body quantum systems is still under debate (4, 7–10).

Although the dependence of the LW functional on the interaction U was implicit only in the preceding discussion, we may explicitly consider this dependence, including it in our notation as $\Phi[G; U]$. The same convention will be followed for other functionals without comment. As we shall see, unlike the functional $\mathcal{F}[G]$, which diverges at the boundary of S_{++}^n , the LW functional $\Phi[G; U]$ extends continuously to the boundary of G . This relates to the possibility of establishing a diagrammatic expansion $\Phi[G; U]$ with respect to the interaction strength.

So far we have considered the LW formalism for any interaction that satisfies the strong growth condition. To draw a closer connection with the diagrammatic expansion used in quantum

many-body physics, we now restrict our attention to the quartic interaction

$$U(x) = \frac{1}{8} \sum_{i,j=1}^n v_{ij} x_i^2 x_j^2. \quad [10]$$

Here $v_{ij} = v_{ji}$ is symmetric, and the symmetry factor 8 simplifies the counting when deriving diagrammatic approximations. v should be chosen so that the corresponding U satisfies the strong growth condition. In particular, this condition is satisfied if $v_{ij} \geq 0$ for all i, j , with strict inequality holding for $i = j$. The interaction Eq. 10 can mimic a short-range interaction as well as a long-range (such as Coulomb) interaction in its second quantized form (13). One can derive an exact correspondence between the Feynman diagrammatic expansions in this lattice field theory and those in condensed matter physics (11), neglecting the particle-hole distinction.

For fixed interaction U and $G \in \mathcal{S}_{++}^n$, we may define a perturbative expansion of $\Phi[G; \varepsilon U]$ with respect to the interaction strength ε . *Theorem 3* shows that the bold diagrammatic expansion of the LW functional at G can be understood as the asymptotic series in ε for the LW functional at G . Note that for the series in Eq. 11 to be asymptotic means that the error of the N th partial sum is $O(\varepsilon^{N+1})$ as $\varepsilon \rightarrow 0$. The importance of *Theorem 3* is to show that the bold diagrammatic expansion is well defined without any reference to the noninteracting Green's function G_0 .

Theorem 3 (Bold Diagrammatic Expansion). *For any interaction $U: \mathbb{R}^n \rightarrow \mathbb{R}$ satisfying the strong growth condition, the LW functional and the self-energy have the following asymptotic series expansions:*

$$\Phi[G; \varepsilon U] = \sum_{k=1}^{\infty} \Phi^{(k)}[G; U] \varepsilon^k, \quad \Sigma[G; \varepsilon U] = \sum_{k=1}^{\infty} \Sigma^{(k)}[G; U] \varepsilon^k. \quad [11]$$

Moreover, for U of the form Eq. 10, the coefficients of the asymptotic series satisfy

$$\Phi^{(k)}[G; U] = \frac{1}{2k} \text{Tr} \left[G \Sigma^{(k)}[G; U] \right], \quad [12]$$

and $\Sigma^{(k)}[G; U]$ consists of all one-particle irreducible skeleton diagrams of order k .

For example, when the U dependence is determined by v_{ij} as in Eq. 10, one can show that the self-energy obtained from bold diagrammatic expansion up to second order is

$$\begin{aligned} \left(\Sigma^{(1)}[G] \right)_{ij} &= -\frac{1}{2} \left(\sum_k v_{ik} G_{kk} \right) \delta_{ij} - v_{ij} G_{ij}, \\ \left(\Sigma^{(2)}[G] \right)_{ij} &= \frac{1}{2} G_{ij} \left(\sum_{k,l} v_{ik} G_{kl}^2 v_{lj} \right) + \sum_{k,l} v_{ik} G_{kj} G_{kl} G_{li} v_{jl}. \end{aligned}$$

For readers familiar with Feynman diagrams, the corresponding diagrams (or graphs) are given in Fig. 1. (See, e.g., ref. 11 for

a general discussion.) In each graph, a vertex connected only to a truncated thin line is called an external vertex and represents the i or j index of the self-energy matrix. All other vertices are internal vertices, which are to be summed over in the expansion. Each “bold” line (represented as a double line) connecting two internal vertices labeled as k, l represents the Green's function G_{kl} . When the bold line forms a closed circle, it is interpreted as the diagonal element G_{kk} . Each wiggled line connecting two internal vertices labeled as k, l represents the interaction $-v_{kl}$. The factor $\frac{1}{2}$ is associated with the symmetry factor of the graph.

Compared with the Feynman diagrams for condensed matter systems, we find that not coincidentally, Fig. 1A and B corresponds to the Hartree and Fock exchange diagrams, respectively, and Fig. 1C and D corresponds to the ring and second-order exchange diagrams, respectively. The only difference is that the lines in the diagrams in Fig. 1 do not possess directions, due to the absence of any distinction between creation and annihilation operators.

Interestingly, the relation Eq. 12 was originally assumed to be true to obtain a formal derivation of the LW functional (1, 22). Our proof here does not rely on such formal manipulation, but instead only on the transformation rule (*Proposition 4*) below and the quartic nature of the interaction U .

Finally, we remark that certain properties in the Euclidean setting, such as the concavity of the free energy functional, can noticeably fail in the non-Euclidean setting. Indeed, the original setting for the LW formalism is a field theory described by the fermionic coherent state path integral represented by Grassmann variables. The free energy functional is nonconcave and the induced Legendre correspondence may not be one to one. This leads to the failure of the LW formalism observed in refs. 4 and 7–10, and the full picture of the LW functional remains to be revealed. Intriguingly, the LW formalism may also be seen as an expansion of a static density matrix formalism (16, 19), which itself does enjoy convexity properties and hence well-defined Legendre duality. However, the density matrix formalism is not induced in the same way by a field theory and does not enjoy even formally properties such as the diagrammatic expansion. The Euclidean field theory setting can then be viewed as combining the best of both worlds, in that it enjoys the convexity properties needed for the nonperturbative definition of the Legendre dual functionals, as well as the formal properties convenient for systematic approximation as in diagrammatic expansions and DMFT.

This work also opens up several immediate research directions. By making a connection between quantum many-body physics and Euclidean lattice field theory, it lowers the barrier for quantitatively assessing the effectiveness of bold diagrammatic schemes and other numerical schemes based on many-body perturbation theory such as the GW theory (2). Possible topics to be developed include the effectiveness of self-consistent many-body perturbation theories and the effectiveness of the vertex correction methods in the GW theory. Theoretical properties of impurity models and embedding schemes, such as the DMFT, can also be studied in the context of Euclidean lattice field theory using the LW formalism.

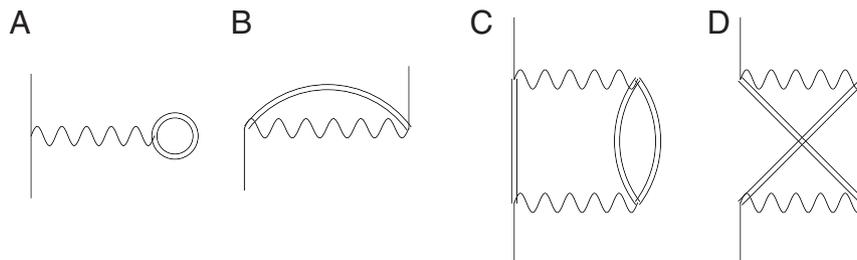


Fig. 1. Bold diagrams for the first-order (A and B) and second-order (C and D) contribution to the self-energy for interaction of the form Eq. 10.

Outline of the proof of Theorem 1: First, we reformulate the computation of the Gibbs free energy $\Omega[A] = -\log Z[A]$ as a minimization problem:

$$\Omega[A] = \inf_{\rho \in \mathcal{M}} \left[\int \left(\frac{1}{2} x^T A x + U(x) \right) \rho dx - S(\rho) \right]. \quad [13]$$

This is the classical Gibbs variational principle (23). For a short proof adapted to this setting, see *Proof of the Classical Gibbs Variational Principle in Theorem 1*.

Next, we split the infimum in Eq. 13 as

$$\Omega[A] = \inf_{G \in \mathcal{S}_{++}^n} \left(\frac{1}{2} \text{Tr}[AG] + \inf_{\rho \in \mathcal{G}^{-1}(G)} \left[\int U \rho dx - S(\rho) \right] \right). \quad [14]$$

Here we have used $\int x^T A x \rho dx = \text{Tr}[\mathcal{G}(\rho)A]$. By introducing the functional Eq. 5, we obtain the variational formulation in Eq. 4. Now Eq. 4 means precisely that Ω is the Legendre dual or more precisely the concave conjugate of \mathcal{F} with respect to the inner product $\langle A, G \rangle = \frac{1}{2} \text{Tr}[AG]$. This is denoted by $\Omega = \mathcal{F}^*$.

One can further prove that \mathcal{F} is concave on \mathcal{S}_{++}^n and diverges to $-\infty$ at the boundary of \mathcal{S}_{++}^n (*Proof That \mathcal{F} Is Concave in Theorem 1* and *Proof That \mathcal{F} Diverges to $-\infty$ at the Boundary of \mathcal{S}_{++}^n in Theorem 1*). Based on these facts, we have that $\mathcal{F} = \mathcal{F}^{**}$; i.e., $\mathcal{F} = \Omega^*$, so \mathcal{F} and Ω are concave duals of one another. Furthermore, it can be shown using the strict concavity and C^∞ smoothness of $\Omega = \mathcal{F}^*$ that \mathcal{F} is strictly concave and C^∞ smooth on \mathcal{S}_{++}^n .

The Legendre duality suggests that $\nabla \mathcal{F}$ and $\nabla \Omega$ are inverses of one another; i.e., the mapping $G[A] := \nabla \Omega[A]$ is a bijection $\mathcal{S}^n \rightarrow \mathcal{S}_{++}^n$, with inverse given by $A[G] := \nabla \mathcal{F}[G]$. Moreover, we remark that for any $G \in \mathcal{S}_{++}^n$, the supremum in the definition Eq. 5 of $\mathcal{F}[G]$ is uniquely attained at the probability density $\rho_G(x) := \frac{1}{Z[A[G]]} e^{-\frac{1}{2} x^T A[G] x - U(x)}$.

Q.E.D.

Outline of the proof of Theorem 2: The differentiability of the LW functional on \mathcal{S}_{++}^n directly follows from the C^∞ -smooth property of $\mathcal{F}[G]$ on \mathcal{S}_{++}^n . Hence the self-energy $\Sigma[G] = \nabla \Phi[G]$ is well defined on \mathcal{S}_{++}^n . Using the LW functional, Eq. 4 can be written as

$$\Omega[A] = \frac{1}{2} \inf_{G \in \mathcal{S}^n} (\text{Tr}[AG] - \text{Tr}[\log(G)] - \Phi[G] - \Phi_0). \quad [15]$$

The Euler–Lagrange equation with respect to G gives the Dyson equation Eq. 8, and the uniqueness of the solution follows from that of the minimizer in *Theorem 1*.

We now establish that unlike $\mathcal{F}[G]$, which blows up at the boundary of \mathcal{S}_{++}^n , the LW functional $\Phi[G]$ extends continuously to the boundary of \mathcal{S}_{++}^n , so in fact the LW functional is well defined on \mathcal{S}_+^n . We first state a useful property of the LW functional, which relates a basis transformation of the Green’s function with a transformation of the interaction (*Proof of the Transformation Rule (Proposition 4)*).

Proposition 4 (Transformation Rule). *Let $G \in \mathcal{S}_{++}^n$, and let U be the interaction term. Let T denote an invertible matrix in $\mathbb{R}^{n \times n}$, as well as the corresponding linear transformation $\mathbb{R}^n \rightarrow \mathbb{R}^n$. Then*

$$\Phi[TGT^*; U] = \Phi[G; U \circ T].$$

Using the transformation rule, we need only to specify a formula for computing $\Phi[G]$ for matrices of the form $G = \begin{pmatrix} G_p & 0 \\ 0 & 0 \end{pmatrix}$ with $G_p \in \mathcal{S}_{++}^p$, $p \leq n$. Indeed, any matrix $G \in \mathcal{S}_+^n$ with rank $p \leq n$ can be represented as such after an appropriate change of basis, so together with the transformation rule, such a formula will pin down the value of $\Phi[G]$ for all $G \in \mathcal{S}_+^n$.

Define a p -dimensional interaction $U_p: \mathbb{R}^p \rightarrow \mathbb{R}$ by the rule $U_p(\cdot) = U(\cdot, 0)$. We prove that

$$\Phi_n[G; U] = \Phi_p[G_p; U_p] \quad [16]$$

defines the continuous extension of Φ_n to the boundary of \mathcal{S}_{++}^n . Here Φ_n and Φ_p are the LW functionals for the n -dimensional and p -dimensional lattice field theories, respectively. We sketch the proof of this fact in *Sketch of the Proof of the Continuous Extension of the LW Functional in Theorem 2*.

Q.E.D.

Outline of the proof of Theorem 3: For a given Green’s function G and interaction U , for notational simplicity we omit the dependence on G and U from the notation via the definitions $\Phi(\varepsilon) := \Phi[G; \varepsilon U]$ and $\Sigma(\varepsilon) = \Sigma[G; \varepsilon U]$. We first prove that there exists an asymptotic series of the form Eq. 11. This existence proof is nonconstructive, and hence the series coefficients still need to be determined. We abbreviate the notation for the series coefficients via $\Phi^{(k)} := \Phi^{(k)}[G; U]$ and $\Sigma^{(k)} := \Sigma^{(k)}[G; U]$. Here the superscript (k) is just a notation and does not indicate the k th-order derivative.

Theorem 3 then consists of identifying that these coefficients are given by the bold diagrammatic expansion using G and U . Our strategy is to first evaluate the expansion for the self-energy and then pin down the coefficients for the LW functional by proving the relation Eq. 12. Since the series expansion is valid only in the asymptotic sense, for any finite ε we consider the truncation at finite-order N , which is denoted by $\bar{\Sigma}^{(N)}(\varepsilon) := \sum_{k=0}^N \Sigma^{(k)} \varepsilon^k$. Then we have $\Sigma(\varepsilon) - \bar{\Sigma}^{(N)}(\varepsilon) = O(\varepsilon^{N+1})$. For the purpose of this discussion, $O(\varepsilon^{N+1})$ will be thought of as negligibly small.

A difficulty in proving *Theorem 3* is that, although we wish to use the technique that resums bare self-energy diagrams to bold self-energy diagrams, $\Sigma[G; \varepsilon U]$ is defined without reference to any bare propagator. *Lemma 5* below identifies a bare propagator $G_0^{(N)}(\varepsilon)$ that generates (up to negligible error) the bold propagator G under the interaction εU . The rest of the proof involves rigorous resummation of the diagrams using $G_0^{(N)}(\varepsilon)$ up to finite order to obtain the bold diagrammatic expansion (*Proof of the Resummation Step in Theorem 3*). After this, the relation Eq. 12 is a consequence of the transformation rule (*Proof of the Expansion Coefficients of the LW Functional in Theorem 3*).

It remains to introduce the aforementioned *Lemma 5* and explain how it allows us to identify a bare propagator (dependent on ε) that generates G under the interaction εU , up to negligible error. *Lemma 5* says that $\bar{\Sigma}^{(N)}(\varepsilon)$ can be identified as the exact self-energy with respect to a modified interaction term (*Proof of Lemma 5*):

Lemma 5. $\bar{\Sigma}^{(N)}(\varepsilon)$ is the self-energy at G induced by the modified interaction $U_\varepsilon^{(N)}(x) := \varepsilon U(x) + \frac{1}{2} x^T (\Sigma(\varepsilon) - \bar{\Sigma}^{(N)}(\varepsilon)) x$. In other words, $\bar{\Sigma}^{(N)}(\varepsilon) = \Sigma[G; U_\varepsilon^{(N)}]$ is the exact self-energy corresponding to a noninteracting Green’s function

$$G_0^{(N)}(\varepsilon) := \left(G^{-1} + \bar{\Sigma}^{(N)}(\varepsilon) \right)^{-1} \quad [17]$$

and the interaction $U_\varepsilon^{(N)}$.

Note carefully that *Lemma 5* is a nonperturbative fact and is valid for all $\varepsilon > 0$. In a perturbative context, since $\bar{\Sigma}^{(N)}(\varepsilon)$ is the self-energy yielded exactly by the bare propagator $G_0^{(N)}(\varepsilon)$ under the interaction $U_\varepsilon^{(N)}$, and since $U_\varepsilon^{(N)}(x)$ (for any given x) differs from $\varepsilon U(x)$ by negligible error, one expects that the self-energy $\bar{\Sigma}^{(N)}(\varepsilon)$ yielded exactly by the same bare propagator under the

interaction εU differs from $\bar{\Sigma}^{(N)}(\varepsilon)$ by only negligible error, and this is indeed true.

Then one finds, by swapping $\bar{\Sigma}$ out for $\tilde{\Sigma}$ in Eq. 17, that

$$\tilde{G}^{(N)}(\varepsilon) := \left(\left[G_0^{(N)}(\varepsilon) \right]^{-1} - \tilde{\Sigma}^{(N)}(\varepsilon) \right)^{-1} \approx G,$$

in the sense that equality holds with negligible error. But $\tilde{G}^{(N)}(\varepsilon)$ is precisely the bold propagator generated by the bare propagator $G_0^{(N)}(\varepsilon)$ under interaction εU . This bold propagator then

matches G up to negligible error as claimed. Together with the resummation step (*Proof of the Resummation Step in Theorem 3*), this establishes the expansion for the self-energy.

Q.E.D.

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