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Bold diagrammatic Monte Carlo study of φ^4 theory

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By incorporating renormalization procedure into bold diagrammatic Monte Carlo, we propose a method for studying quantum field theories in the strong coupling regime. Bold diagrammatic Monte Carlo essentially samples Feynman diagrams using local Metropolis-type updates. Applying the method to three-dimensional φ^4 theory, we analyze the strong coupling limit of the theory and confirm the existence of a nontrivial IR fixed point in agreement with prior studies. Interestingly, we find that working with bold correlation functions as building blocks of the Monte Carlo procedure renders the scheme convergent, and no further resummation method is needed.

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Lattice field theory is a well-established approach for nonperturbative studies in quantum field theories. This is based on the Euclidean path integral formulation of quantum field theory and a stochastic sampling of the partition function. This method has played a central role in developing our understanding of strongly coupled systems including quantum chromodynamics in particle physics and quantum many-body systems in condensed matter physics. However, the severe sign problem is a main obstacle in applying lattice methods to systems at finite chemical potential or calculating transport coefficients in the thermodynamic limit.

A different method based on diagrammatic formulation of field theory has been developed in the last few years, called diagrammatic Monte Carlo [1–3]. The basic idea is to perform a Monte Carlo process in the space of Feynman diagrams using local Metropolis-type updates. Unlike lattice field theory, the diagrammatic Monte Carlo samples physical quantities in the thermodynamic limit, which washes out systematic errors produced by finite size effects. However, because of the divergence of the perturbation series, one usually needs a resummation technique to make the scheme convergent. This method has been applied successfully to several systems including the polaron problem [2] and the Fermi–Hubbard model [4]. In particular, using the Borel resummation technique, the triviality of the φ^4 theory in four and five dimensions as well as the instability of the trivial fixed point in three dimensions were established in Ref. [5].

One way of improving the convergence of the diagrammatic Monte Carlo scheme is to expand physical quantities in terms of full screened (bold) correlation functions, instead of free correlators, as is usually done in field theory. This method, known as bold diagrammatic Monte Carlo (BDMC), is shown to have a broader range of convergence [6]. Interestingly, using BDMC, the sign problem becomes an advantage for the convergence of the scheme. A recent BDMC implementation for a strongly interacting fermionic system, namely, unitary Fermi gas, shows an excellent agreement with experimental results on trapped ultracold atoms [7]. In particular, the equation of state of the system at finite chemical potential has been studied, which is hard to achieve by lattice methods due to the sign problem.

In this paper, by incorporating the renormalization procedure into the BDMC scheme, we propose a method for studying relativistic quantum field theories in the strong coupling regime. The method is generic and applicable to any renormalizable quantum field theory. We apply the method to φ^4 theory in three dimensions with the bare action

$$S_b = \int d^3x \left\{ \frac{1}{2}\varphi_b(x)(-\partial^2 + m_0^2)\varphi_b(x) + \frac{g_0}{4!}\varphi_b^4(x) \right\},$$

where m_0 and g_0 are the bare mass and coupling, respectively. It is more economical to use the notation of Ref. [12] and rewrite the action as

$$S_b = \frac{1}{2}\int_{12} G_{12}^{-1}\varphi_1\varphi_2 + \frac{1}{4!}\int_{1234} V_{1234}\varphi_1\varphi_2\varphi_3\varphi_4,$$

where the spatial arguments are indicated by number indices. The kernel G^{-1} and potential V are given by

$$G_{12}^{-1} \equiv G^{-1}(x_1, x_2) = (-\partial_{x_1}^2 + m^2)\delta(x_1 - x_2),$$
$$V_{1234} \equiv \delta(x_1 - x_2)\delta(x_1 - x_3)\delta(x_1 - x_4).$$

This model has a nontrivial IR fixed point, first shown by Wilson and Fisher [8], using the ϵ expansion and renormalization group techniques. According to the renormalization group (RG) arguments [9–11], renormalized coupling, g_r, tends to a fixed value, g_r^*, when bare coupling becomes very large, $g_0 \to \infty$. Therefore, any nonperturbative numerical approach to quantum field theory (QFT) should be able to demonstrate this feature of the theory.

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We show that the renormalized BDMC technique allows us to go beyond perturbative regime and find the fixed point. Interestingly, we find that working with bold correlation functions as building blocks of the Monte Carlo scheme renders the scheme convergent, and no further resummation method is needed.

Our starting point is a set of Schwinger–Dyson equations for bare self-energy, Σ_b, and bare one-particle irreducible four-point functions, $\Gamma_b^{(4)}$, derived in Ref. [12]. The basic idea is to consider a Feynman diagram as a functional of its elements, like propagator lines. Differentiation with respect to the free propagator, G_b, leads to a set of Schwinger–Dyson equations for correlation functions. Using this method, one finds [12]

$$\Sigma_{b,12} = -\frac{1}{2}\int_{34} V_{b,1234}\boldsymbol{G}_{b,34} + \frac{1}{6}\int_{345678} V_{b,1345}\boldsymbol{G}_{b,36}\boldsymbol{G}_{b,47}\boldsymbol{G}_{b,58}\boldsymbol{\Gamma}_{b,6782} \tag{1}$$

$$\boldsymbol{\Gamma}_{b,1234} = V_{b,1234} + \tilde{\mathcal{A}}_{b,1234} + \tilde{\mathcal{B}}_{b,1234} + \mathcal{C}_{b,1234}, \tag{2}$$

in which a tilde means a partial permutation on indices

$$\tilde{\mathcal{A}}_{b,1234} = \mathcal{A}_{b,1234} + \mathcal{A}_{b,1324} + \mathcal{A}_{b,1423},$$
$$\tilde{\mathcal{B}}_{b,1234} = \mathcal{B}_{b,1234} + \mathcal{B}_{b,1324} + \mathcal{B}_{b,1423},$$

with

$$\mathcal{A}_{b,1234} = -\frac{1}{2}V_{b,1256}\boldsymbol{G}_{b,57}\boldsymbol{G}_{b,68}\boldsymbol{\Gamma}_{b,7834},$$
$$\mathcal{B}_{b,1234} = +\frac{1}{6}V_{b,5167}\boldsymbol{G}_{b,69}\boldsymbol{G}_{b,70}\boldsymbol{\Gamma}_{b,902\bar{1}}\boldsymbol{G}_{b,\bar{1}\bar{2}}\boldsymbol{\Gamma}_{b,\bar{2}348}\boldsymbol{G}_{b,85},$$
$$\mathcal{C}_{b,1234} = -\frac{1}{3}V_{b,1567}\boldsymbol{G}_{b,58}G_{b,69}G_{b,70}\frac{\delta\Gamma_{b,8234}}{\delta G_{b,90}}.$$

From now on, integration over repeated indices is understood. The advantage of this set of equations is that all terms on the right-hand sides of Eqs. (1) and (2) are one-particle irreducible, and therefore no irrelevant diagram will be produced during the Monte Carlo simulation. Also, all terms are expressed in terms of bold (exact) correlation functions except the derivative term, $\mathcal{C}_b$, in Eq. (2). To increase the efficiency of the method, we rewrite this term using the functional chain rule and the identity

$$\boldsymbol{G}^{c}_{1234} = -2\frac{\delta\boldsymbol{G}_{12}}{\delta G^{-1}_{34}} - \boldsymbol{G}_{13}\boldsymbol{G}_{24} - \boldsymbol{G}_{14}\boldsymbol{G}_{23}, \tag{3}$$

where $\boldsymbol{G}^{c}_{1234}$ is the connected four-point function. We end up with the following bold representation of the derivative term

$$\mathcal{C}_{b,1234} = \mathcal{D}_{b,1234} + \bar{\mathcal{D}}_{b,1234}, \tag{4}$$

with

$$\mathcal{D}_{b,1234} = -\frac{1}{3}V_{b,1567}\boldsymbol{G}_{b,58}\boldsymbol{G}_{b,69}\boldsymbol{G}_{b,70}\frac{\delta\Gamma_{b,8234}}{\delta\boldsymbol{G}_{90}},$$
$$\bar{\mathcal{D}}_{b,1234} = +\frac{1}{6}V_{b,1567}\boldsymbol{G}_{b,58}\boldsymbol{G}_{b,6\bar{1}}\boldsymbol{G}_{b,7\bar{2}}\boldsymbol{G}_{b,9\bar{3}} \cdot\boldsymbol{G}_{b,0\bar{4}}\boldsymbol{\Gamma}_{b,\bar{1}\bar{2}\bar{3}\bar{4}}\frac{\delta\Gamma_{b,8234}}{\delta\boldsymbol{G}_{90}}.$$

A diagrammatic representation of Eqs. (1) and (2) is illustrated in Fig. 1.

By differentiating the one-particle irreducible (1PI) vertex function, Eq. (2), with respect to the full propagator, $\boldsymbol{G}$, we find series expansions in terms of bold correlation functions for the self-energy and vertex function, in a recursive way. In particular, for the first derivative, we have

$$\frac{\delta\Gamma_{b,1234}}{\delta\boldsymbol{G}_{b,\alpha\beta}} = -\frac{1}{2}V_{b,12\alpha6}\boldsymbol{G}_{b,68}\boldsymbol{\Gamma}_{b,8\beta34} + \alpha\leftrightarrow\beta + \cdots,$$

where dots stand for higher-order terms (higher order in terms of the number of bold propagators). We find that approximating the derivative term by the first term is sufficient for finding the fixed point.To study the behavior of the renormalized coupling constant, we translate the

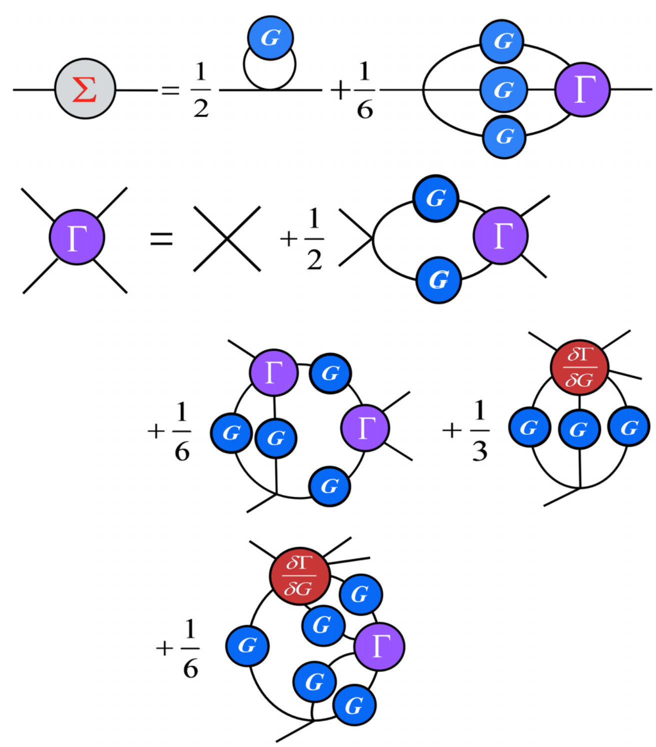

FIG. 1 (color online). Bold diagrammatic expansions for the self-energy and one-particle irreducible vertex function in φ^4 theory. All diagrams on the right-hand sides are individually one-particle irreducible and expressed in terms of exact propagators.

Schwinger–Dyson equations into equations for renormalized correlation functions and impose renormalization conditions

$$\boldsymbol{\Gamma}_r^{(2)}(p^2 = 0) = m^2 \tag{5}$$

$$\frac{\partial}{\partial p^2}\Gamma_r^{(2)}(p^2)|_{p^2=0} = 1 \tag{6}$$

$$\boldsymbol{\Gamma}_r^{(4)}(0,0,0,0) = m^{4-d} g_r. \tag{7}$$

The renormalized proper two-point function, which satisfies Eqs. (5) and (6), can be written as

$$\boldsymbol{\Gamma}_r^{(2)}(p^2) \equiv \boldsymbol{G}_r^{-1}(p^2) = Z(p^2 + \mathbf{Y}(p^2)) + m^2, \tag{8}$$

where $\mathbf{Y}(p^2) = \Sigma_b(p^2 = 0) - \Sigma_b(p^2)$ and the field renormalization constant is given by

$$Z = \frac{1}{1 + \frac{\partial \mathbf{Y}(p^2)}{\partial p^2}\Big|_{p^2=0}}. \tag{9}$$

Using Eq. (1), one may rewrite $\mathbf{Y}(p^2)$ in terms of renormalized quantities as

$$\mathbf{Y}(p^2) = \frac{g_0 Z}{6}\int \frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}\boldsymbol{G}_r(k)\boldsymbol{G}_r(q) \times [\boldsymbol{G}_r(Q)\boldsymbol{\Gamma}_r^{(4)}(0,\vec{k},\vec{q},\vec{Q}) - \boldsymbol{G}_r(Q)\boldsymbol{\Gamma}_r^{(4)}(\vec{p},\vec{k},\vec{q},\vec{Q})], \tag{10}$$

where in each term the momentum $\vec{Q}$ is determined by the conservation of momenta that appear in the vertex function argument. The φ^4 theory in three dimensions is super-renormalizable and has only three superficially divergent diagrams, all eliminated by the mass counterterm. In addition $\mathbf{Y}(p^2)$ is finite in any order of perturbation. Furthermore, all vertex diagrams are superficially finite, and we find that it is useful to work with the bare form of the Schwinger–Dyson equation (2) in this case; however, we have to replace bare two-point functions with the renormalized ones.

Our strategy for computing the renormalized coupling constant corresponding to a given bare coupling is to solve coupled Schwinger–Dyson equations (2) and (10) by means of general BDMC rules, starting with the tree-level approximation for correlation functions. After reaching convergence, the renormalized coupling constant can be read off from Eq. (7) by recalling that $\boldsymbol{\Gamma}_r^{(4)} = Z^2\Gamma_b^{(4)}$.

To increase the efficiency of the algorithm, inspired by the idea of the worm algorithm [13] and following Ref. [14], instead of sampling the $\mathbf{Y}(p)$ and $\boldsymbol{\Gamma}_b^{(4)}$ directly, we introduce two auxiliary normalization constant terms and sample the quantities

$$I_2 = \alpha_2 + \int \mathbf{Y}(p^2)\Omega(p)^2 dp \tag{11}$$

$$I_4 = \alpha_4 + \int \boldsymbol{\Gamma}_b^{(4)}(p_1, p_2, p_3, \chi_{12}, \chi_{13}, \chi_{23}) d\mathbf{X}, \tag{12}$$

with $d\mathbf{X} = dp_1 dp_2 dp_3 d\chi_{12} d\chi_{13} d\chi_{23}$, where χ_{ij} is the cosine of the angle between $\vec{p}_i$ and $\vec{p}_j$ and $\Omega(p)$ is the normalized probability density that we use to generate new momenta in Monte Carlo updates. We skip the details of the Monte Carlo procedure and report the results here.

Figure 2 depicts the renormalized coupling constant as a function of the bare coupling. As is evident from this plot, g_r tends to an asymptotic value in accordance with the renormalization group prediction. Also, the value of the fixed point, $\tilde{g}_r^* = \frac{3}{16\pi} g_r^* = 1.40 \pm 0.05$, agrees, within error, with the high-temperature series expansion and resummed ϵ expansion [10,11]. It is worth noticing that Fig. 2 provides a nonperturbative calculation of φ^4 theory based on summing up Feynman diagrams. This plot interpolates between weak and strong coupling regimes, and indeed it is not possible to produce such a result by using just perturabtive methods or RG techniques.

It is also interesting to calculate critical exponents by using the BDMC method. Since critical exponents are related to the scaling behavior of composite operators, we construct a new set of Schwinger–Dyson equations for diagrammatic expansion of composite operators in

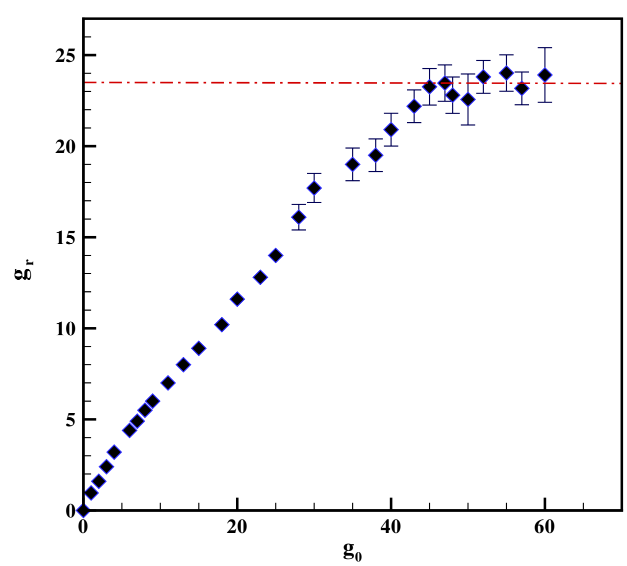

FIG. 2 (color online). Result of bold diagrammatic Monte carlo simulation for dimensionless renormalized coupling constant, g_r, as a function of bare coupling. The asymptotic behavior of renormalized coupling is in agreement with the existence of an IR fixed point.

terms of bold correlators. For example, the critical exponent ν, which controls the growth of correlation length near the phase transition, is related to the IR behavior of the composite operator with one φ^2 insertion, $\Gamma^{(1,2)}$. It is straightforward to derive coupled equations for $\mathbf{\Gamma}^{(1,2)}$ and $\mathbf{\Gamma}^{(1,4)}$ from Eqs. (1) and (2) by using the mass derivative trick for generating correlation functions with φ^2 insertions

$$\Gamma_b^{(1,2)}(0,p) = 1 - \frac{\partial}{\partial m^2}\Sigma_b(p)$$

$$\mathbf{\Gamma}_b^{(1,4)}(0,p) = \frac{\partial}{\partial m^2}\Gamma_b^{(4)}(p).$$

Turning on BDMC machinery, it is straightforward to solve this new set of equations in a similar way as discussed for Eqs. (1) and (2). We postpone the numerical implementation to future works.

In summary, we described a nonperturbative simulation of a relativistic QFT, φ^4 theory in three dimensions, based on sampling bold Feynman diagrams. We used a set of coupled Schwinger–Dyson equations to expand physical quantities in terms of exact correlation functions. The systematic method of deriving such bold expansions in quantum field theories was proposed in Ref. [15] and used to construct connected Feynman diagrams and to calculate their corresponding weights in φ^4 theory [12] and quantum electrodynamics [16]. It is based on this fact that a complete knowledge of vacuum energy implies the knowledge of all scattering amplitudes; "vacuum is the world" [17].

In addition, in renormalizable QFTs, it is always possible to formulate such Schwinger–Dyson equations in terms of renormalized correlation functions and finite integrals. Combining with the BDMC technique to sample unknown functions in terms of them, this offers a universal scheme for nonperturbative calculations in QFTs.

Applying this approach to non-Abelian gauge theories is under progress, however, one may need more complicated resummation methods to recover the correct physical values from truncated bold expansions. In the case of φ^4 theory, interestingly, we observed that without using any resummation technique truncating the series at lowest order leads to convergent results.

One way to reduce systematic errors produced by the truncation of bold series is introducing a complete basis of functions and expanding correlation functions in terms of them, $\boldsymbol{G}_{12} = \sum_{n,m} c_{n,m}\psi_{n,1}\psi_{m,2}$. By considering $\mathbf{\Gamma}^{(4)}$ as a function of $c_{n,m}$ coefficients, the functional derivative term takes the following form:

$$\frac{\delta\Gamma^{(4)}_{1234}}{\delta\boldsymbol{G}_{56}} = \sum_{n,m}\frac{\partial\mathbf{\Gamma}_{8234}}{\partial c_{n,m}}\psi_{n,5}\psi_{m,6}. \tag{13}$$

Performing a Monte Carlo process in the space of $c_{n,m}$ coefficients to sample the derivative term increases the accuracy of the algorithm drastically.

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