Bold Diagrammatic Monte Carlo Study of $\phi^4$ Theory

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By incorporating renormalization procedure into Bold Diagrammatic Monte Carlo (BDMC), we propose a method for studying quantum field theories in the strong coupling regime. BDMC essentially samples Feynman diagrams using local Metropolis-type updates and does not suffer from the sign problem. Applying the method to three dimensional $\phi^4$ 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 non-perturbative 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 chromodynamic 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 (DMC) [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, DMC samples physical quantities in the thermodynamic limit which washes out systematic errors produced by finite size effects. However due to divergence of perturbation series, one usually needs a resummation technique to make the scheme convergent. This method has been applied successfully to several systems including polaron problem [2] and the Fermi-Hubbard model [4]. In particular using the Borel resummation technique, triviality of the $\phi^4$ theory in four and five dimensions as well as instability of trivial fixed point in three dimensions have been established in [5].

One way of improving the convergence of 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 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 sign problem.

In this Letter, by incorporating renormalization procedure into Bold Diagrammatic Monte Carlo (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. This provides a new computational toolbox for studying longstanding problems in high energy physics, where implementing lattice approach suffers from the sign problem.

We apply the method to $\phi^4$ theory in three dimensions with the following bare action

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

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

$$S_b = \frac{1}{2} \int_{12} G_{12}^{-1} \phi_1 \phi_2 + \frac{1}{4!} \int_{1234} V_{1234} \phi_1 \phi_2 \phi_3 \phi_4 ,$$

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

$$G_{12}^{-1} = G^{-1}(x_1, x_2) = (-\partial^2_1 + m^2) \delta(x_1 - x_2),$$

$$V_{1234} = \delta(x_1 - x_2) \delta(x_1 - x_3) \delta(x_1 - x_4).$$

This model has a nontrivial IR fixed point, first shown by Wilson and Fisher [8], using the $\epsilon$ expansion and renormalization group techniques. According to the RG
arguments \cite{9,11}, renormalized coupling, \( g_r \), tends to a fixed value, \( g_r^* \), when bare coupling becomes very large, \( g_0 \rightarrow \infty \). Therefore any non-perturbative numerical approach to QFT, should be able to demonstrate this feature of the theory. 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 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, \( \Sigma_b \), and bare one-particle irreducible four point functions, \( \Gamma_b^{(4)} \), derived in \cite{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 \cite{12}

\[
\Sigma_{b,12} = -\frac{1}{2} \int_{34} V_{b,1234} G_{b,34} + \frac{1}{6} \int_{345678} V_{b,134567} G_{b,36} G_{b,47} G_{b,58} \Gamma_{b,6782} \tag{1}
\]

\[
\Gamma_{b,1234} = V_{b,1234} + \tilde{A}_{b,1234} + \tilde{B}_{b,1234} + c_{b,1234} , \tag{2}
\]

in which tilde means a partial permutation on indices

\[
\tilde{A}_{b,1234} = A_{b,1234} + A_{b,1324} + A_{b,1423} ,
\]

\[
\tilde{B}_{b,1234} = B_{b,1234} + B_{b,1324} + B_{b,1423} ,
\]

with

\[
A_{b,1234} = -\frac{1}{2} V_{b,1256} G_{b,57} G_{b,68} \Gamma_{b,7834} ,
\]

\[
B_{b,1234} = +\frac{1}{6} V_{b,1567} G_{b,69} G_{b,70} \Gamma_{b,9021} G_{b,12} \Gamma_{b,2348} G_{b,85} ,
\]

\[
c_{b,1234} = -\frac{1}{3} V_{b,1567} G_{b,58} G_{b,69} G_{b,70} \frac{\delta \Gamma_{b,8234}}{\delta G_{b,90}} .
\]

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 (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, \( c_b \), in (2). To increase the efficiency of the method we rewrite this term using the functional chain rule and the following identity

\[
G_{1234} = -2 \frac{\delta G_{12}}{\delta G_{34}} - G_{13} G_{24} - G_{14} G_{23} , \tag{3}
\]

where \( G_{1234} \) is the connected four point function. We end up with the following bold representation of the derivative term

\[
\frac{\delta \Gamma_{b,1234}}{\delta G_{b,\alpha\beta}} = -\frac{1}{2} V_{b,12a6} G_{b,68} \Gamma_{b,834} + \alpha \rightarrow \beta + \cdots ,
\]

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

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

\[
\frac{\delta \Gamma_{b,1234}}{\delta G_{b,\alpha\beta}} = \frac{1}{6} \frac{\delta \Gamma_{b,1234}}{\delta G_{b,\alpha}} + \frac{1}{3} \frac{\delta \Gamma_{b,1234}}{\delta G_{b,\beta}} .
\]
fies (5) and (6) can be written as

\[ \Gamma_r^{(2)}(p^2 = 0) = m^2 \]  
\[ \frac{\partial}{\partial p^2} \Gamma_r^{(2)}(p^2)|_{p^2=0} = 1 \]  
\[ \Gamma_r^{(4)}(0, 0, 0, 0) = m^{4-d} g_r. \]

The renormalized proper 2-point function which satisfies (5) and (6) can be written as

\[ \Gamma_r^{(2)}(p^2) \equiv G_r^{-1}(p^2) = Z \left( p^2 + Y(p^2) \right) + m^2, \]

where \( Y(p^2) = \Sigma_0(p^2 = 0) - \Sigma_0(p^2) \) and the field renormalization constant is given by

\[ Z = \frac{1}{1 + \frac{\partial Y(p^2)}{\partial p^2}|_{p^2=0}}. \]

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

\[ Y(p^2) = \frac{g_b Z}{6} \int \frac{d^3k}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} G_r(k) G_r(q) \]
\[ \times \left[ G_r(Q) \Gamma_r^{(4)}(0, k^\perp, q^\perp, Q^\perp) - G_r(Q) \Gamma_r^{(4)}(p^\perp, k^\perp, q^\perp, Q^\perp) \right], \]

where in each term the momentum \( Q^\perp \) is determined by the conservation of momenta that appear in the vertex renormalization argument. The \( \phi^4 \) theory in 3 dimensions is super-renormalizable and has only three superficially divergent diagrams, all eliminated by the mass counter term. In addition, \( Y(p^2) \) 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, renormalized coupling constant can be read off from (7) by recalling that \( \Gamma_r^{(4)} = Z^2 \Gamma_b^{(4)} \).

In order to increase the efficiency of the algorithm, inspired by the idea of worm algorithm \[13\] and following \[14\], instead of sampling the \( Y(p) \) and \( \Gamma_b^{(4)} \) directly, we introduce two auxiliary normalization constant terms and sample the following quantities

\[ I_2 = \alpha_2 + \int Y(p^2) \Omega(p)^2 \, dp \]  
\[ I_4 = \alpha_4 + \int \Gamma_b^{(4)}(p_1, p_2, p_3; \chi_{123}) \, dX \]

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

Fig. 2 depicts the renormalized coupling constant as a function of 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, \( \tilde{g}_r = 3.8 g_b = 1.40 \pm 0.05 \), agrees, within error, with the high temperature series expansion and resummed \( \epsilon \)-expansion \[10, 11\]. It is worth noticing that Fig. 2 provides a non-perturbative calculation of \( \phi^4 \) 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 perturbative 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

\[ \frac{\partial}{\partial p^2} \Gamma_r^{(2)}(p^2)|_{p^2=0} = 1 \]  
\[ \Gamma_r^{(4)}(0, 0, 0, 0) = m^{4-d} g_r. \]

The 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.

![Figure 2: Result of Bold diagrammatic Monte Carlo simulation for dimensionless renormalized coupling constant, g_r as a function of bare coupling.](image-url)
diagrammatic expansion of composite operators in terms of bold correlators. For example the critical exponent \(\nu\), which controls the growth of correlation length near the phase transition, is related to the IR behavior of the composite operator with one \(\phi^2\) insertion, \(\Im^{(1,2)}\). It is straightforward to derive coupled equations for \(\Im^{(1,2)}\) and \(\Im^{(1,4)}\) from [1] and [2] by using the mass derivative trick for generating correlation functions with \(\phi^2\) insertions.

\[
\Im_b^{(1,2)}(0, p) = 1 - \frac{\partial}{\partial m^2} \Sigma_b(p)
\]

\[
\Im_b^{(1,4)}(0, p) = \frac{\partial}{\partial m^2} \Im_b^{(4)}(p).
\]

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

**Conclusions and outlook.** In summary we described a non-perturbative simulation of a relativistic QFT, \(\phi^4\) theory in 3-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 [15] and used to construct connected Feynman diagrams and to calculate their corresponding weights in \(\phi^4\) 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 QFT’s it is always possible to formulate such Schwinger-Dyson equations in terms of renormalized correlation functions and finite integrals. Combining with BDMC technique to sampling unknown functions in terms of them, this offers a universal scheme for non-perturbative calculations in QFT’s.

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

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

\[
\frac{\delta \Im^{(4)}_{\alpha 23}^{14}}{\delta G_{56}} = \sum_{n,m} \frac{\partial \Phi_{8234}^{56}}{\partial c_{n,m}} \psi_{n,5} \psi_{m,6} .
\]

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

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