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Beyond the Variational Principle in Quantum Field Theory

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Abstract

A method of summing diagrams in quantum field theory beyond the variational Gaussian approximation is proposed using the continuum form of the recently developed plaquette expansion. In the context of $\lambda\phi^4$ theory the Hamiltonian, $H[\phi]$, of the Schrödinger functional equation $H[\phi]\Psi[\phi] = E\Psi[\phi]$ can be written down in tri–diagonal form as a cluster expansion in terms of connected moment coefficients derived from Hamiltonian moments $\langle H^n\rangle \equiv \int \mathcal{D}\phi V_1[\phi]H^n[\phi]V_1[\phi]$ with respect to a trial state $V_1[\phi]$. The usual variational procedure corresponds to minimising the zeroth order of this cluster expansion. At first order in the expansion, the Hamiltonian in this form can be diagonalised analytically. The subsequent expression for the vacuum energy E contains Hamiltonian moments up to fourth order and hence is a summation over multi-loop diagrams, laying the foundation for the calculation of the effective potential beyond the Gaussian approximation.

1. Introduction

There has been much effort over the years devoted to the problem of summation of diagrams in continuum quantum field theory defined in four-dimensional space–time. Achieving a full non-perturbative solution in the continuum is usually seen as a hopeless task and has been totally abandoned by many in favour of Monte Carlo simulation of lattice regularised theories. The few long-standing methods that are capable of summing over particular classes of diagrams include renormalisation group, Schwinger–Dyson equations, $1/N$ expansions and the variational principle. In each case the ability to extend the summation to larger classes of diagrams is severely limited and hence there are many efforts at finding alternative schemes. The requirements are simple to state—an approximation scheme is sought carrying out summation over classes of diagrams which can be improved systematically without impossible effort to achieve convergence of physical results.

In this paper a candidate method satisfying these requirements is proposed. This method is based on the analytic cluster expansion property (Hollenberg 1993) of the Lanczos tri–diagonalisation procedure formulated in the functional Schrödinger picture. The method reduces to the usual variational principle at zeroth order and thus represents a systematic improvement of the variational method.

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2. The $\lambda\phi^4$ Theory in the Functional Schrödinger Picture

To illustrate we will consider $\lambda\phi^4$ theory, the Lagrangian of which is given by

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi - \tfrac{1}{2}m^2\phi^2 - \lambda\phi^4 . \tag{1}$$

In the Schrödinger functional formalism the equal time commutation relation (Rosen 1968)

$$[\phi(\boldsymbol{x}), \pi(\boldsymbol{y})] = i\delta(\boldsymbol{x} - \boldsymbol{y}) \tag{2}$$

is satisfied by the replacement

$$\pi(\boldsymbol{x}) \to i\frac{\delta}{\delta\phi(\boldsymbol{x})} , \tag{3}$$

so that the Hamiltonian becomes

$$H[\phi] = \int \mathrm{d}\boldsymbol{x}\{-\tfrac{1}{2}\frac{\delta^2}{\delta\phi(\boldsymbol{x})^2} + \tfrac{1}{2}(\nabla\phi(\boldsymbol{x}))^2 + \tfrac{1}{2}m^2\phi(\boldsymbol{x})^2 + \lambda\phi(\boldsymbol{x})^4\} . \tag{4}$$

The functional operator $H[\phi]$ acts on state functionals $\Psi[\phi]$ for which the functional Schrödinger equation is

$$H[\phi]\Psi[\phi] = E\Psi[\phi] . \tag{5}$$

The solution to the free theory vacuum in this formalism is simply the Gaussian functional

$$\Psi_{(\lambda=0)}[\phi] = \mathcal{N}\exp\{-\tfrac{1}{2}\int \mathrm{d}\boldsymbol{x}\,\phi(\boldsymbol{x})\sqrt{m^2 - \nabla^2}\,\phi(\boldsymbol{x})\} , \tag{6}$$

where $\mathcal{N}$ is a normalisation constant. Traditionally, the variational treatment of the $\lambda \neq 0$ theory starts with a Gaussian trial state (Barnes and Ghandour 1980)

$$\Psi_F[\phi] = \mathcal{N}_F\exp\{-\tfrac{1}{2}\int \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}\,\phi(\boldsymbol{x})F(\boldsymbol{x} - \boldsymbol{y})\,\phi(\boldsymbol{y})\} . \tag{7}$$

The function $F(\boldsymbol{x} - \boldsymbol{y})$ is determined by minimising the energy functional $E_{\mathrm{var}}[F]$ given by the expectation value

$$E_{\mathrm{var}}[F] = \int \mathcal{D}\phi\Psi_F[\phi]H[\phi]\Psi_F[\phi] . \tag{8}$$

The variationally minimised energy $E_{\mathrm{var}}[F]$ is a summation over all 'bubble' diagrams. The purpose of this work is to describe a method by which one can systematically sum over increasing classes of diagrams beyond that of the Gaussian approximation.

3. Lanczos Cluster Expansion in the Continuum

In principle, the exact vacuum energy (and spectrum), summing over all classes of diagrams, can be obtained by diagonalisation of the functional Schrödinger equation. This task is of course beyond present means, however, it is useful to consider the solution of the functional Schrödinger equation by diagonalisation in the light of approximation methods for such problems in many-body theory. In particular, the recently formulated plaquette expansion method (Hollenberg 1993) for approximately diagonalising lattice Hamiltonians in the infinite-volume limit is well suited to this problem.

The application of this approximation scheme to the diagonalisation of the functional Schrödinger equation proceeds in the same manner as for the lattice many-body problem. Starting with an initial state $V_1[\phi]$ (e.g. $V_1[\phi] = \Psi_{(\lambda=0)}[\phi]$ or $V_1[\phi] = \Psi_F[\phi]$) a basis of states $\{V_n[\phi]\}$ is constructed according to the Lanczos recursion

$$V_n[\phi] = \frac{1}{\beta_{n-1}}\left[(H[\phi] - \alpha_{n-1})V_{n-1}[\phi] - \beta_{n-2}V_{n-2}[\phi]\right], \tag{9}$$

where $\alpha_n = \int \mathcal{D}\phi V_n[\phi]H[\phi]V_n[\phi]$ and $\beta_n = \int \mathcal{D}\phi V_{n+1}[\phi]H[\phi]V_n[\phi]$. At the nth iteration of this recursion the Hamiltonian matrix T_n is

$$T_n = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix} \tag{10}$$

Diagonalisation of the matrices T_n for increasing n gives converging upper bounds to the energy spectrum of the original Hamiltonian. In terms of the initial state, the calculation of the exact matrix at the nth iteration requires calculation of the Hamiltonian moments up to $\langle H^{2n-1}\rangle = \int \mathcal{D}\phi V_1[\phi]H^{2n-1}[\phi]V_1[\phi]$. This is the approach taken by Choe *et al.* (1988) in their application of the analytic Lanczos method to lattice field theory. Since Hamiltonian moments are in general difficult to calculate, one is limited to only the first few exact Lanczos iterations and the large-volume limit cannot be taken. Progress can be made via a cluster expansion of the Lanczos recursion which makes optimal use of the lowest moments. This is precisely the plaquette expansion, which relies on the fact that the *connected* Hamiltonian moments $\langle H^n\rangle_c$ are extensive in the number of plaquettes N_p (or volume) on the lattice, i.e. $\langle H^n\rangle_c \propto N_p$. One of the main points of this paper is that this extensive property of the many-body lattice problem carries over to the continuum field-theoretic problem and hence the Lanczos cluster expansion can be applied to the diagonalisation of the Schrödinger functional equation.

Specifically, given an appropriate trial state $V_1[\phi]$ whose *connected* Hamiltonian moments (i.e. cumulants) scale with the volume Ω as $\langle H^n\rangle_c = c_n\Omega$, the Lanczos recursion admits expansions for α_n and β_n of the form (Hollenberg 1993)

$$\alpha_n = \Omega c_1 + (n-1)\left[\frac{c_3}{c_2}\right] + \tfrac{1}{2}(n-1)(n-2)\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{2c_2^4}\right]\frac{1}{\Omega} + \dots ,$$

$$\beta_n^2 = nc_2\Omega + \tfrac{1}{2}n(n-1)\left[\frac{c_2c_4 - c_3^2}{c_2^2}\right]$$

$$+ \tfrac{1}{6}n(n-1)(n-2)\left[\frac{-12c_3^4 + 21c_2c_3^2c_4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{2c_2^5}\right]\frac{1}{\Omega} + \dots . \tag{11}$$

It can be seen immediately that the connected moment coefficients c_n, derived from the Hamiltonian moments $\langle H^n \rangle = \int \mathcal{D}\Phi V_1[\Phi] H^n[\Phi] V_1[\Phi]$, correspond to diagrams of increasing complexity and hence the expansion systematically includes larger classes of diagrams weighted appropriately with the volume. Diagonalisation of the tri–diagonal matrix in this approximate form sums over the classes of diagrams represented by the expansion order. This is a converging procedure in the limit $\Omega \to \infty$, as has been explicitly demonstrated for various lattice examples. Systematic increase in the class of diagrams is achieved by increasing the order of the expansion.

Here we are interested in the analytic insight one may glean from summation of diagrams beyond the Gaussian approximation and so the numerical possibilities, important as they are, will not immediately concern us. At our disposal is the fact that the tri–diagonal matrix at first order in the expansion (i.e. up to the $1/\Omega$ term) can be diagonalised analytically. In the large-volume limit the lowest eigenvalue (i.e. the vacuum energy if the appropriate trial state has been used) is given by (Hollenberg and Witte 1994)

$$E_0 = \Omega\left[c_1 + \frac{c_2^2}{c_2c_4 - c_3^2}\{\sqrt{3c_3^2 - 2c_2c_4} - c_3\}\right] . \tag{12}$$

The presence of the c_4 term indicates that the above expression represents a summation over diagrams up to and including those contained in $\langle H^4 \rangle$. The exact class of diagrams summed over depends on the trial state used.

For renormalisation purposes, the preferred option might be to calculate moments with respect to a shifted Gaussian (Barnes and Ghandour 1980)

$$\Psi_{\phi_0}[\phi] = \mathcal{N}\exp\{-\tfrac{1}{2}\int \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}\,(\phi(\boldsymbol{x}) - \phi_0)F_{\phi_0}(\boldsymbol{x} - \boldsymbol{y})\,(\phi(\boldsymbol{y}) - \phi_0)\}\,, \tag{13}$$

from which the *Gaussian* effective potential (Stevenson 1984, 1985; Barnes and Ghandour 1980) is calculated as

$$V_{\mathrm{eff}}^{(\mathrm{Gauss})}(\phi_0) = \min\left[\int \mathcal{D}\phi\Psi_{\phi_0}[\phi]H[\phi]\Psi_{\phi_0}[\phi]\right] . \tag{14}$$

The Gaussian effective potential coincides with minimising the zeroth order of the Lanczos cluster expansion, calculated from the shifted Gaussian trial state,

with respect to the function $F_{\phi_0}(\boldsymbol{x}-\boldsymbol{y})$. Since the first-order expression from the Lanczos cluster expansion, E_0, sums over a larger class of diagrams, it is much closer to the ground state energy than the variational result. Hence, one would expect that the effective potential would be much better approximated by the *Lanczos effective potential* which we define as

$$V_{\text{eff}}^{(\text{Lanczos})}(\phi_0) = V_{\text{eff}}^{(\text{Gauss})}(\phi_0) + \Omega\,\frac{c_2(\phi_0)^2\,[\sqrt{3c_3(\phi_0)^2 - 2c_2(\phi_0)c_4(\phi_0)} - c_3(\phi_0)]}{c_2(\phi_0)c_4(\phi_0) - c_3(\phi_0)^2}\,, \tag{15}$$

where the connected moments $c_n(\phi_0)$ (suppressing dependence on the bare parameters m and λ) are calculated with respect the minimised shifted Gaussian trial state; i.e. the first moment is

$$c_1(\phi_0) = \frac{1}{\Omega} V_{\text{eff}}^{(\text{Gauss})}(\phi_0)\,. \tag{16}$$

The advantage of calculating in the framework of the effective potential is the relative ease with which renormalisation of the bare parameters, λ and m, can be carried out—as has been shown to be the case for $V_{\text{eff}}^{(\text{Gauss})}(\phi_0)$ (Stevenson 1985).

Table 1. First-order Lanczos cluster expansion approximation, $E_0(\lambda)$, for the ground state of the anharmonic oscillator, $H = -\frac{1}{2}\,\mathrm{d}^2/\mathrm{d}x^2 + \frac{1}{2}\,x^2 + \lambda x^4$

$\log_{10}\lambda$	Variational	$E_0(\lambda)$	Exact
0	0·8125	0·8037	0·8038
1	1·5313	1·5040	1·5050
2	3·1924	3·1286	3·1314
3	6·8280	6·6877	6·6942
4	14·6871	14·3838	14·3980
5	31·6317	30·9775	31·0103
6	68·1434	66·7338	67·0993

The calculation of the moments to fourth order in $\lambda\phi^4$ field theory is a reasonable algebraic challenge and is currently being undertaken. However, an indication of the improvement over the variational calculation which might be obtained is given in Table 1 for the case of the anharmonic oscillator (Hollenberg *et al.* 1993). The variationally minimised Gaussian trial state is used as the trial state for the Lanczos cluster expansion. The accuracy of the first-order Lanczos cluster expansion is typically a factor of *ten* better than the variational calculation. It is hoped that this significant improvement of the variational calculation carries over to the field-theoretic case.

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