Coupled-cluster renormalization group

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Abstract
The coupled cluster method (CCM) is one of the most successful and universally applicable techniques in quantum many-body theory. The intrinsic nonlinear and non-perturbative nature of the method is considered to be one of its advantages. We present here a combination of CCM with the Wilsonian renormalization group which leads to a powerful framework for construction of effective Hamiltonian field theories. As a toy example we obtain the two-loop renormalized $\phi^4$ theory.

1. INTRODUCTION
The CCM originated in nuclear physics around forty years ago on the work of Coester and Kümmel [1]. There exists several versions of CCM formulation [2]. They are denoted generically as independent-cluster (IC) parametrizations, in the sense that they incorporate the many-body correlations via sets of amplitudes that describe various correlated clusters within the interacting system as mutually independent entities. The IC methods differ in the way they incorporate the locality and separability properties. Each of the IC methods has been shown to provide an exact mapping of the original quantum mechanical problem to a corresponding classical mechanics in terms of a set of multiconfigurational canonical field amplitudes. In this way one can introduce a particular differentiable IC manifold which is endowed with a symplectic structure. The basic IC amplitudes provide the local coordinates on these manifold.

Despite extensive studies of the CCM in different areas of physics, limited progress has been made in application of the CCM to modern particle physics [3]. In the recent paper [4, 5] we showed that the implementation of the Wilsonian exact renormalization group approach in the CCM framework leads to an elegant method for obtaining Hamiltonian renormalization flows. Our method resembles the similarity renormalization group [6] (see the talk by Glazek), since we employ a double non-unitary transformation (using the extended CCM) to decouple the irrelevant degrees of freedom, which leads to partial diagonalization of the Hamiltonian. In this note we present a short review of our approach.

2. FORMALISM
Notice that our formulation does not depend on the form of the dynamics (i.e. equal time or light cone). We assume that generally the renormalized Hamiltonian $H_{\text{eff}}(\lambda)$ up to scale $\lambda$ can be expressed as

$$H_{\text{eff}}(\lambda) = H(\lambda) + H_C(\lambda),$$

where $H_C(\lambda)$ is a “counterterm”. Now we introduce a large cut-off $\Lambda$. We define two subspaces, the model-space $P : \{ |L\rangle \otimes |0, b\rangle_h, L \leq \mu \}$ and the complement-space $Q : \{ |L\rangle \otimes (|H\rangle - |0, b\rangle_h), \mu < H \leq \Lambda \}$. The ket $|0, b\rangle_h$ is the bare high-energy vacuum (the ground state of the free high-momentum Hamiltonian). The $P$-space contains interacting low-energy states and the $Q$-space contains the orthogonal complement (the symbols $|L\rangle$ and $|H\rangle$ denote generic low- and high-energy states, respectively). Our renormalization approach is based on decoupling of the complement space $Q$ from the model space $P$ by using a non-unitary transformation aiming at constructing of the counterterms. The transformation of $H(\Lambda)$ is defined by

$$\mathcal{P} = e^{\hat{S}(\mu, \Lambda)} e^{-\hat{S}(\mu, \Lambda)} H(\Lambda) e^{\hat{S}(\mu, \Lambda)} e^{-\hat{S}(\mu, \Lambda)} \equiv H(\mu) + \delta H(\mu, \Lambda),$$

(2)
and we can expand $\hat{S}(\hat{S}')$ in terms of the independent coupled cluster excitation $I$, assuming a naive power counting.

$$\hat{S} = \sum_{m=0} \hat{S}_m \left( \frac{\mu}{\lambda} \right)^m,$$

$$\hat{S}' = \sum_{m=0} \hat{S}'_m \left( \frac{\mu}{\lambda} \right)^m,$$

$$\hat{S}_m = \sum_l s_l C_l^\dagger,$$

$$\hat{S}'_m = \sum_l s'_l C_l. \tag{3}$$

Here the primed sum means that $I \neq 0$, and momentum conservation is included in $s_l$ and $s'_l$. The $C_l$ and $C_l^\dagger$ are annihilation and creation operators in the high-energy Fock space for the chosen quantization scheme. The indices $I$ define a subsystem, or cluster, within the full system of a given configuration. Notice that $s_l$ and $s'_l$ are parameters in the high-energy Fock space, while they are operators in the low-energy Fock space. Therefore one can guarantee the proper size-extensivity and conformity with the linked-cluster theorem (at any level of approximation) in the Wilsonian high-energy shell. However one can still apply the standard CCM parametrization after obtaining the effective low-energy Hamiltonian (thus the size-extensivity can be extended to the whole Fock space).

It is well-known in CCM formulation that the parametrization Eq. (3) is compatible with the Hellmann-Feynman theorem and the phase space $\{s_l, s'_l\}$ for a given $m$ is a symplectic differentiable manifold. Having said that, the representation in this way can no longer remain manifestly hermitian. This in fact give rise to some superfluous degrees of freedom since the actual phase space is enlarged into a complex manifold. There is long tradition for such approaches, of course with different motivation (e.g., in the BRST formalism, the phase space is expanded by anti-commuting canonical coordinates). As Arponen emphasized [7] the most important reason behind the extra degrees of freedom in the CCM is the fact that one can introduce a universal average value functional allowing the simultaneous computation of the expectations of other operators than the Hamiltonian. In Ref. [5] we showed that this non-unitarity leads to an economic computation and does not induce any relevant non-hermiticity in the renormalization group sense. On the other hand this can, in principle, lead to Poincaré invariance at any given level of truncation regardless of the regularization scheme. One may now impose the decoupling conditions derivable from the dynamics of the quantum system, leading to diagonalization of the transformed Hamiltonian matrix (double similarity transformation splits diagonalization to upper and lower triangle part),

$$Q\Pi P = 0 \rightarrow \langle 0 | C_l e^{-\hat{S}} H e^{\hat{S}} | 0 \rangle = 0, \tag{4}$$

$$P\Pi Q = 0 \rightarrow \langle 0 | e^{\hat{S}'} e^{-\hat{S}} H e^{\hat{S}} e^{-\hat{S}'} C_l^\dagger | 0 \rangle = 0, \tag{5}$$

where $I \neq 0$. Thus the effective low-energy Hamiltonian is

$$\hat{H}_{\text{eff}} = P\Pi P \equiv \frac{1}{\hbar} \langle b, 0 | e^{\hat{S}(\mu, \Lambda)} e^{-\hat{S}(\mu, \Lambda)} H(\Lambda) e^{\hat{S}(\mu, \Lambda)} e^{-\hat{S}(\mu, \Lambda)} | 0, b \rangle_h. \tag{6}$$

The decoupling conditions Eqs. (4,5) make the $P$ sector of the truncated Fock space independent of the rest. This means that the contribution of the excluded sector of Hilbert space (the high-energy space) is taken into account by imposing the decoupling conditions. These are sufficient requirements to secure partial diagonalization of the Hamiltonian in the fast-particle space. This technique seems to be more universal than Wilsonian renormalization based on Lagrangian framework since one can eliminate other irrelevant degrees of freedom in a unified way.

Here, by construction, the energy-dependent Bloch-Feshbach formalism is made free of the small-energy denominators which plague perturbation theory. One can then determine the counterterm by requiring coupling coherence [8], namely that the transformed Hamiltonian Eq. (6) has the same form given in Eq. (1), with $\lambda$ replaced by $\mu$. By means of the decoupling conditions one can determine the unknown individual amplitudes $s_l$ and $s'_l$ for a given $m$ in a consistent truncation scheme which is the
so-called SUB($n,m$). The choice of $n$ depends on the bare Hamiltonian interaction and should be fixed from the outset.

The formulation is intrinsically non-perturbative, however we can simply apply a perturbation expansion. We split the Hamiltonian in five parts: $H = H_1 + H_2^{\text{free}}(\text{high}) + V_C(C_1^i) + V_A(C_i) + V_B$ where $H_1$ contains only the low frequency modes with $k \leq \mu$, $H_2$ is the free Hamiltonian for all modes with $\mu < k < \Lambda$, $V_C$ contains low frequency operators and products of the high frequency creation operators $C_i^d$ and $V_A$ is the hermitian conjugate of $V_C$. The remaining terms are contained in $V_B$. If we assume that $V_{A,C,B}$ are of first order in coupling constant, then one can expand Eqs. (4) in order of $m$, leading to the elimination of the fast-particle up first order in the coupling. This produces an effective Hamiltonian up to third order in the coupling:

$$
m = 0 : \langle 0 | C_I (V_C + [H_2, \hat{S}_0]) | 0 \rangle = 0,
= \langle 0 | (V_A - [H_2, \hat{S}_0]) C_I^d | 0 \rangle = 0,

m = 1 : \langle 0 | C_I ([H_1, \hat{S}_0] + [H_2, \hat{S}_1] + [V_A, \hat{S}_1] + [V_C, \hat{S}_1]) | 0 \rangle = 0,
= \langle 0 | ([H_1, \hat{S}_0] + [H_2, \hat{S}_1] + [V_C, \hat{S}_1] + [V_A, \hat{S}_1] - [V_A, \hat{S}_1]) C_I^d | 0 \rangle = 0,

m = n : \langle 0 | C_I ([H_1, \hat{S}_{n-1}] + [H_2, \hat{S}_n] + [V_A, \hat{S}_n] + [V_C, \hat{S}_n]) | 0 \rangle = 0,
= \langle 0 | ([H_1, \hat{S}_{n-1}] + [H_2, \hat{S}_n] + [V_C, \hat{S}_n] + [V_A, \hat{S}_n] - [V_A, \hat{S}_n]) C_I^d | 0 \rangle = 0. \tag{7}

3. EXAMPLE

We now apply this formalism to the computation of the effective Hamiltonian for $\phi^4$ theory up to two-loop order in equal-time quantization. The details can be found in Ref. [5]. The bare $\phi^4$ theory Hamiltonian is

$$
H = \int d^3 x \left( \frac{1}{2} \pi^2(x) + \frac{1}{2} \phi(x) ( - \nabla^2 + m^2 ) \phi(x) + g \phi^4(x) \right). \tag{8}
$$

We now split field operators into high- and low-momentum modes; $\phi(x) = \phi_L(x) + \phi_H(x)$, where $\phi_L(x)$ denotes modes of low-frequency with momentum $k \leq \mu$ and $\phi_H(x)$ denotes modes of high-frequency with momentum constrained to a shell $\mu < k < \Lambda$. The $\phi_H(x)$ is represented in the Fock space as $\phi_H(x) = \sum_{k < \mu} \int \frac{d^3 q}{(2\pi)^3} a_k e^{i k x} + a_k^\dagger e^{-i k x}$. One can plug this expansion into Eq. (8) and produce the Fock representation of the Hamiltonian (in the high-energy space), the high-energy configurations in the Fock space are specified by $\{C_I \to \prod_{k=1}^{16} a_k \}$ and $\{C_I^d \to \prod_{k=1}^{16} a_k^\dagger \}$. Up to two-loop expansion, our renormalization scheme requires us to keep $S(S')$ at least to order $n = 4$. The $\hat{S}(\hat{S})$ operators consistent with a $SUB(4,m)$ truncation scheme are,

$$
\hat{S}_m = \sum \left( \hat{S}_m^1 a_k^\dagger \hat{S}_m^2 a_k^\dagger a_p^\dagger + \hat{S}_m^3 a_k^\dagger a_p^a q^\dagger + \hat{S}_m^4 a_k^\dagger a_p^a q^\dagger a_r^\dagger \right),
\hat{S}_m' = \sum \left( \hat{S}_m'^1 a_k + \hat{S}_m'^2 a_k a_p + \hat{S}_m'^3 a_k a_p a_q + \hat{S}_m'^4 a_k a_p a_q a_r \right). \tag{9}
$$

The unknown coefficients $\hat{S}_m(\hat{S}_m')$ in Eq. (9) can be found by Eqs. (4,5) or Eq. (7). We restrict ourselves to the elimination of the high-energy degrees of freedom up to first order in the coupling constant $g$ and in a consistent truncation scheme $SUB(4,2)$. For $m = 0$, the potential divergent terms arise from

$$
\delta H = \langle 0 | H + [H, \hat{S}_0^{(3)}] + [H, \hat{S}_0], \hat{S}_0^d | 0 \rangle = \frac{3g}{4\pi^2} \langle \Lambda^2 - \mu^2 \rangle \int d^3 x \phi^2(x)
\quad - \frac{9g^2}{2\pi^2} \ln \left( \frac{\Lambda}{\mu} \right) \int d^3 x \phi^4(x) - \frac{3g^2}{2\pi^4} (2 \ln 2 - 1) \Lambda^2 \int d^3 x \phi^2(x)
\quad + \frac{3g^2}{16\pi^4} \ln \left( \frac{\Lambda}{\mu} \right) \int d^3 x (\nabla \phi(x))^2 + \frac{27g^4}{2\pi^4} \left[ \left( \ln \left( \frac{\Lambda}{\mu} \right) \right)^2 + \ln \left( \frac{\Lambda}{\mu} \right) \right] \int d^3 x. \tag{10}
$$
One can immediately deduce the renormalization factors $Z_m$, $Z_g$ and $Z_\phi$ from the above equation,

$$Z_m = 1 - \frac{3g^2}{2\pi^2}(\Lambda^2 - \mu^2), \quad Z_\phi = 1 - \frac{3g^2}{8\pi^4} \ln \left( \frac{\Lambda}{\mu} \right).$$

$$Z_g = 1 + \frac{9g^2}{2\pi^2} \ln \left( \frac{\Lambda}{\mu} \right) + \frac{g^3}{4\pi^4} \left( 81 \left( \ln \left( \frac{\Lambda}{\mu} \right) \right)^2 - 51 \ln \left( \frac{\Lambda}{\mu} \right) \right).$$

(11)

In the same way one can obtain the unknown coefficients for $m = 1$. The only divergent contribution up to order $g^2$ arises from

$$\delta H = -\langle 0 | [H_1, \hat{S}_1] | \hat{S}_0 \rangle | 0 \rangle = -\frac{3g^2}{16\pi^4} \ln \left( \frac{\Lambda}{\mu} \right) \int d^3 x \pi^2(x),$$

(12)

which contributes to the two-loop wave-function renormalization $Z_\pi$, namely it leads to $Z_\pi = Z_\phi^{-1}$. One now may reproduce the well-known two-loop $\beta$- and $\gamma$-functions by making use of Eq. (11).

4. CONCLUSION

In this note we have outlined a strategy to construct effective Hamiltonian field theories in framework of well-known coupled cluster many body theory. We showed that this method has several advantages: 1: all other irrelevant degrees of freedom like many-body states can be systematically eliminated in the same way, 2: renormalization flows can be obtained perturbatively or non-perturbatively. 3: the formulation is free of any small-energy denominator plaguing old-fashion perturbation theory, 4: with the implementation of the decoupling properties, having the phase space extended to a complex manifold, one can in principle preserve Poincaré invariance regardless of a regularization scheme, 5: the formulation is not restricted to any quantization scheme (e.g. equal time or light cone).

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References

[1] F. Coester, Nucl. Phys. 7, 42 (1957); F. Coester and H. Kümmel, Nucl. Phys. 17, 477 (1960).

[2] R. F. Bishop, Theor. Chim. Acta. 80, 95 (1991); in Lecture notes in physics, Vol. 510, Springer, Berlin, p.1 (1997) and references therein.

[3] See for example: U. Kaulfuss, Phys. Rev. D32, 6, 1421 (1985); G. Hasberg and H. Kümmel, Phys. Rev. C33, 1367 (1986); H. Kümmel, Phys. Rev. D50, 6556 (1993); N. E. Ligerink, N. R. Walet and R. F. Bishop, Ann. Phys. (N.Y.) 267, 97 (1998); 284, 215 (2000); A. P. Szczepaniak and P. Krupinski, Phys. Rev. D66, 096006 (2002).

[4] A. H. Rezaeian and N. R. Walet, [hep-ph/0212196].

[5] A. H. Rezaeian and N. R. Walet, Phys. Lett. B570, 129 (2003).

[6] S. D. Glazek and K. G. Wilson, Phys. Rev. D48, 5863 (1993); F. Wegner, Ann. Physik (Berlin) 3, 77 (1994).

[7] J. Arponen, Phys. Rev. A55, 2686 (1997).

[8] R. J. Perry and K. G. Wilson, Nucl. Phys. B403, 587 (1993); R. Oehme, K. Sibold and W. Zimmermann, Phys. Lett. B147, 115 (1984).