Renormalization of Hamiltonians

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This paper presents a new renormalization procedure for Hamiltonians such as those of light-front field theory. The bare Hamiltonian with an arbitrarily large, but finite cutoff, is transformed by a specially chosen similarity transformation. The similarity transformation has two desirable features. First, the transformed Hamiltonian is band diagonal: in particular, all matrix elements vanish which would otherwise have caused transitions with big energy jumps, such as from a state of bounded energy to a state with an energy of the order of the cutoff. At the same time, neither the similarity transformation nor the transformed Hamiltonian, computed in perturbation theory, contain vanishing or near-vanishing energy denominators. Instead, energy differences in denominators can be replaced by energy sums for purposes of order of magnitude estimates needed to determine cutoff dependences. These two properties make it possible to determine relatively easily the list of counterterms needed to obtain finite low energy results (such as for eigenvalues). A simple model Hamiltonian is discussed to illustrate the method.

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I. INTRODUCTION

Light-front field theory raises very complex renormalization issues. Furthermore, traditional Lagrangian approaches to renormalization do not apply because lightfront field theories are defined instead by their Hamiltonian. This paper explains a new formalism for renormalization of Hamiltonians including determination of the required cutoff-dependent counterterms. Our interest in the formalism is stimulated by its potential applicability to light-front QCD.

The basic reasons for investigating the new method of constructing counterterms in light-front Hamiltonians are the following.

The light-front Fock space description of elementary particles is a natural basis for explaining the Feynman parton model of hadrons. However, this is not yet accomplished because severe divergences appear in lightfront dynamics. There is an urgent need for powerful methods of constructing Hamiltonian counterterms in order to understand the field-theoretical light-front basis of the parton model of hadrons.

The light-front counterterms have complex structure and contain free functions, not just a few free parameters in their finite parts. Physically required values of the functions have to be found in part by fitting experimental data. But, the functions can be severely constrained by symmetry requirements. Full rotational symmetry, which is not explicitly satisfied in the light-front formulation, provides the most powerful constraints. In turn, the counterterms are surely necessary to obtain rotational invariance.

The infrared longitudinal cutoff properties of lightfront theory suggest another fundamental role for the counterterms. Namely, the longitudinal infrared cutoff in light-front dynamics makes it impossible to create particles from a bare vacuum by a translationally invariant Hamiltonian and in addition the number of constituents in a given eigenstate is limited. Light-front counterterms to the longitudinal infrared cutoff dependence become a possible alternative source for features normally associated in standard equal-time dynamics with a nontrivial vacuum structure, including spontaneous symmetry breaking and confinement.

Powerful methods for finding counterterms in lightfront Hamiltonians are necessary to verify these hypotheses. Even if it turns out that the light-front counterterms are not able to solve all problems, we may still learn about why they fail.

We consider a Hamiltonian $H = H_0 + H_I$. H_0 is assumed to be well understood and its eigenstates $|i\rangle$ and corresponding eigenvalues E_i are known. H_I is an interaction which requires a solution. The analysis in perturbation theory of divergences generated from H_I is complicated by the presence of vanishing energy denominators due to nearly degenerate eigenstates of H_0 . These vanishing denominators make it hard to construct upper bounds on complex perturbative formulas, bounds that are useful to separate divergent from convergent terms. At the same time, the terms in H_I that cause the divergences in perturbation theory involve large jumps in energy. The reason for this is that they involve the creation or destruction of high-energy virtual particles in interaction with low energy constituents. A simple 3×3 matrix Hamiltonian in a basis of eigenstates of H_0 will illustrate the problem:

$$H = \begin{bmatrix} \Lambda & g\Lambda & g\Lambda \\ g\Lambda & m & gm \\ g\Lambda & gm & m \end{bmatrix} .$$
(1.1)

<u>48</u> 5863

In this matrix, there are two low-energy degenerate eigenstates of H_0 with eigenvalue *m* and one high-energy state whose eigenvalue Λ defines the cutoff. Then the source of the divergences in such H would be the offdiagonal matrix elements $g\Lambda$ which jump from the energies order m to the energies order Λ , while the source of vanishing energy denominators would be the off-diagonal terms gm between the two degenerate states of energies order m. In this simple case, one would use degenerate perturbation theory for small enough g to compute perturbative corrections to the low-energy states, thereby avoiding any problems with vanishing energy denominators. The question is how to avoid similar problems when one has a field theory with a continuum of energy eigenvalues rather than isolated degenerate subsets as in the example.

In this paper, a formalism will be developed which converts an arbitrary Hamiltonian H to a "banddiagonal" H' so that the "far off-diagonal" terms that are the cause of perturbative divergences will be eliminated. We will give a precise definition of "band-diagonal" later but the intent is that a matrix element H'_{ii} lies in the band if E_i and E_i either are of the same order of magnitude or are both below a threshold energy E_0 . In contrast, a "far off-diagonal" matrix element has $E_i \gg E_j$ or $E_j \gg E_i$ with at least one energy much greater than E_0 . Given a Hamiltonian that is "band diagonal" and where the offdiagonal terms inside the band are treatable by perturbation theory, no ultraviolet divergences can arise in perturbation expansions to any finite order. The reason for this is that if one starts with an external state of fixed energy, and one applies the interaction H'_I of the banded Hamiltonian only a finite number of times to this state, the resulting state has a finite upper bound on the energies it contains and so no divergent integrals (i.e., integrals sensitive to the cutoff Λ) can occur in any finite order of perturbation theory. If a Hamiltonian is "band-diagonal" but its immediate off-diagonal terms within the band are not small enough for perturbation theory to be valid, there can still be nonperturbative divergences. An example is given in Appendix B. We apply our formalism to a simplified model to demonstrate how one can use it to find a generally valid structure of Hamiltonian counterterms in perturbation theory to all orders.

In two previous papers on renormalization-group methods applied to Hamiltonians, a simpler approach to renormalization was used, where all eigenstates of H_0 with energies above a finite bound λ are eliminated, leaving an effective Hamiltonian for the remaining lower energy states [1,2]. (This simpler renormalization-group method was applied to light-front field theory in Ref. [3].) An example of studies of transverse cutoff dependence and low-order counterterms in a light-front Yukawa model can be found in Ref. [4], where one can also find references to the growing literature on light-front theories. A closely related model of the effective Hamiltonian renormalization procedure for transverse lightfront divergences is discussed in Ref. [5]. The mass counterterms in Fock space representation for light-front Hamiltonians are discussed in Ref. [6]. Unfortunately, the simpler effective Hamiltonian approach suffers from

small energy denominators, e.g., the denominators involving differences of the highest energy kept minus the lowest energy eliminated. A need for renormalization procedures in Hamiltonian calculations of the S-matrix elements has been recently exemplified in Refs. [7,8]. Examples of original and review articles which discuss the light-front and closely related infinite momentum frame dynamics can be found in Ref. [9].

The new renormalization formalism is introduced in Sec. II. Section III describes the application to an elementary model. Details of the model analysis to all orders in perturbation theory are given in Appendix A. Section IV concludes the paper. Appendix B provides an example of nonperturbative divergences in a banddiagonal Hamiltonian.

II. SIMILARITY RENORMALIZATION SCHEME

Let us consider a Hamiltonian

$$H = H_0 + H_I \tag{2.1}$$

with a cutoff Λ , where H_I includes both a bare interaction and any necessary counterterms. Strong Λ dependence of the eigenvalues and eigenvectors of H will be generated in perturbation theory unless one has found the structure of the necessary counterterms, because the bare interaction couples states below a fixed energy λ to all states from between λ and Λ with growing strength. The similarity renormalization scheme is based on the observation that if those couplings with large energy jumps were removed, the divergences could not be generated in finite orders of perturbation theory. So, we consider a similarity transformation of the Hamiltonian matrix H such that the transformed Hamiltonian matrix H' has all troublesome elements far away from its diagonal equal zero. A dependence appears in the transformed Hamiltonian in the nonzero matrix elements which are close to diagonal. The cutoff dependence can be removed from these matrix elements by introducing counterterms. The similarity matrix should approach unity when the troublesome interaction is zero, since we work in the basis of eigenstates of H_0 and H_0 is therefore already "band diagonal" too. Similarity transformations preserve eigenvalues and therefore the transformed Hamiltonian H' has the same spectrum as H.

The new Hamiltonian H' is given by the formula

$$H' = S^{-1} HS$$
, (2.2)

where S is the similarity matrix which is unitary, $S^{-1}=S^{\dagger}$. S can be written as

$$S = 1 + T , \qquad (2.3)$$

where $T \rightarrow 0$ when $H_I \rightarrow 0$. Unitarity of S implies that

$$T + T^{\dagger} + T^{\dagger}T = 0 . \qquad (2.4)$$

We introduce two parts of T: the Hermitian $h = \frac{1}{2}(T + T^{\dagger})$, and anti-Hermitian, $a = \frac{1}{2}(T - T^{\dagger})$. Equation (2.4) can be rewritten as

$$h = \frac{1}{2}(a^2 - h^2) . \tag{2.5}$$

Thus, h and a are not independent and h is of higher order in the bare interaction than a.

The new interaction Hamiltonian is defined as $H'_I = H' - H_0$, so that the new free Hamiltonian is the same as the old one and we have

$$H_I' = H_I + T^{\dagger}H + HT + T^{\dagger}HT . \qquad (2.6)$$

Then, we demand that H'_I is "band diagonal," which means that the matrix elements of H'_I which are far away from the diagonal are zero. In order to define what we mean by the matrix elements which are far away from the diagonal we introduce notions of diagonal remotum of a matrix M, denoted DR[M], and diagonal proximum of M, denoted DP[M]. Diagonal proximum refers to the "band-diagonal" part of a matrix and diagonal remotum to the "far off-diagonal" part.

Suppose an operator \hat{M} has matrix elements $M_{ij} = \langle i | \hat{M} | j \rangle$ between the eigenstates of H_0 , $H_0 | i \rangle = E_i | i \rangle$. The indices *i* and *j* run from 0 to some big number determined by the cutoff Λ which defines the size of the matrix *M*. The diagonal remotum of *M* has the same matrix elements as *M* when *i* is far away from *j* in some prescribed way, and the matrix elements $DR[M]_{ij}$ for the close indices *i* and *j* are equal to zero. Then, DP[M] = M - DR[M], i.e., $DP[M]_{ij}$ are the same as M_{ij} when indices *i* and *j* are close to each other in the prescribed way. For example, we may choose

$$\mathbf{DP}[\boldsymbol{M}]_{ij} = \boldsymbol{M}_{ij} \tag{2.7}$$

when

$$|(\beta+1)|E_i - E_j| \le (\beta-1)(E_i + E_j) + 2E_0$$
, (2.8)

where $\beta > 1$, E_i and E_j are the eigenvalues of H_0 (assumed to be positive), and E_0 is some fixed constant. Equation (2.8) implies that (2.7) holds when

$$\beta E_j + E_0 > E_i > \frac{E_j - E_0}{\beta}$$
 (2.9)

Otherwise $DP[M]_{ij}=0$. The above choice removes the possibility that small energy differences appear in the denominators of perturbation theory. This becomes clear in further discussion.

The new interaction Hamiltonian must satisfy the proximity condition

$$H_I' = \mathsf{DP}[H_I'] , \qquad (2.10)$$

which implies the following condition on the similarity matrix through Eq. (2.6):

$$DR[H_{I} + T^{\dagger}H + HT + T^{\dagger}HT] = 0.$$
 (2.11)

This equation may be slightly rewritten

$$DR[H_{I} + \{H_{0}, h\} + [H_{0}, a] + T^{\dagger}H_{I} + H_{I}T + T^{\dagger}HT] = 0,$$
(2.12)

and then satisfied by imposing the following condition on the matrix a:

$$[a, H_0] = \mathbf{DR}(H_I + \{H_0, h\} + T^{\dagger}H_I + H_IT + T^{\dagger}HT) .$$
(2.13)

From this condition we can find the similarity matrix recursively in perturbation theory to all orders in the interaction H_I since we know the eigenstates and eigenvalues of H_0 . The commutator of *a* with H_0 is the lowestorder term in Eq. (2.12) involving the similarity matrix and it may be used to begin the recursion. Then, it follows that

$$H'_{I} = \mathbf{DP}[H_{I} + \{H_{0}, h\} + T^{\dagger}H_{I} + H_{I}T + T^{\dagger}HT]$$
(2.14)

since DP[a]=0 by definition. We observe that the arguments of DR and DP in Eqs. (2.13) and (2.14) are the same. We denote this argument by Q.

For the purpose of carrying out the renormalization program in perturbation theory to all orders we rewrite Qin a different form. Namely, we use the inverse of the similarity relation from Eq. (2.2) and the unitarity condition from Eq. (2.4) to express H_I by H'_I in all terms of Qexcept for the first term which is H_I itself:

$$Q = H_I - \{H_0, h\} + H'_I(a - h) - (a + h)H'_I + (a + h)H'(a - h) .$$
(2.15)

The similarity renormalization scheme is defined recursively in powers of the bare interaction Hamiltonian in the following way.

Let us assume for simplicity that the bare interaction Hamiltonian is proportional to a coupling constant g, with counterterms of higher order:

$$H_I = gV_1 + g^2 V_2 + g^3 V_3 + \cdots . (2.16)$$

 gV_1 is the bare interaction projected on the space limited by the cutoff Λ and V_K for k = 2, 3, ... denote the counterterms. Correspondingly,

$$H_I' = gV_1' + g^2V_2' + g^3V_3' + \cdots$$
 (2.17)

and

$$a = ga_1 + g^2a_2 + g^3a_3 + \cdots . (2.18)$$

The matrix h is of order g^2 ,

$$h = g^2 h_2 + g^3 h_3 + \cdots, \qquad (2.19)$$

where, from Eq. (2.5),

$$h_n = \frac{1}{2} \sum_{k,l;k+l=n} (a_k a_l - h_k h_l) . \qquad (2.20)$$

In order to define the recursion formulas for the counterterms we rewrite Q from Eq. (2.15) as a series in g,

$$Q = gQ_1 + g^2Q_2 + g^3Q_3 + \cdots, \qquad (2.21)$$

so that

5866

STANISŁAW D. GŁAZEK AND KENNETH G. WILSON

Equation (2.22) is our basic result. It is visible that the structure of Q_n is generated by terms involving only V'_k , a_k , and h_k with k < n, except for V_n and one term on the right-hand side of Eq. (2.22) which involves h_n . h_n is expressed by lower-order terms through Eq. (2.20) and V_n completes the definition of Q_n by eliminating the divergent cutoff dependence of other terms. Now, since all V'_k and a_k for $k=1,2,\ldots,n-1$ are generated from $Q_k, k = 1, 2, ..., n - 1$, we have the recursion which expresses Q_n by $Q_k, k = 1, 2, ..., n - 1$. Expression (2.22) for Q_n is designed in such a form, that the counterterm V_n appears in it only once and linearly, added to potentially divergent terms. Thus, the necessary structure of V_n which makes Q_n independent of the big Λ can be determined from the knowledge of finite Q's of lower orders and operators appearing in Eq. (2.22).

Finally, we obtain expressions for V'_n and a_n . Namely,

$$V_n' = \mathbf{DP}[Q_n] \tag{2.23}$$

and

$$a_{nij} = \frac{\mathrm{DR}[Q_n]_{ij}}{E_j - E_i} .$$
(2.24)

This is the only equation which involves energy denominators. Since $DR[Q_n]_{ij}$ vanishes unless E_i and E_j lie outside the band condition from Eq. (2.8) one can verify that

$$|E_i - E_j| > \frac{\beta - 1}{\beta + 1} (E_i + E_j) + \frac{2E_0}{\beta + 1} , \qquad (2.25)$$

which confirms our claim that energy differences are of order their sums.

The induction to all orders in g defines the similarity renormalization scheme in perturbation theory. We are interested in construction of the counterterms V_n for $n = 2, 3, ..., \infty$.

Knowing the generally valid structure of counterterms, one can use Eqs. (2.5), (2.13), and (2.14) to find the new Hamiltonian H' for some values of β and E_0 in Eq. (2.8) in an iterative procedure which is not confined to perturbation theory. In the first approximation one has

$$Q_1 = gV_1$$
 . (2.26)

Neither divergences nor counterterms appear in this case. The first approximation to a new interaction is

$$H_{I1}' = \mathrm{DP}[gV_1]$$
, (2.27)

and the similarity matrix is

$$[a_1, H_0] = \mathbf{DR}[gV_1], \qquad (2.28)$$

together with

$$h_1 = 0$$
 . (2.29)

Thus, the unitarity condition is not manifest in the first approximation. The nonperturbative iterative procedure is defined by

$$Q_{N+1} = H_{I(N+1)} - \{H_0, h_N\} + H'_{IN}(a_N - h_N) - (a_N + h_N)H'_{IN} + (a_N + h_N)H'_N(a_N - h_N) ,$$
(2.30)

where the (N+1)th approximation to the counterterm in $H_{I(N+1)} = gV_1 + V_{N+1}$ is defined to remove all divergences in Q_{N+1} . The complementary recursive relations are

$$H'_{I(N+1)} = \text{DP}[Q_{N+1}],$$
 (2.31)

$$[a_{N+1}, H_0] = \mathbf{DR}[Q_{N+1}], \qquad (2.32)$$

and

$$h_{N+1} = \frac{1}{2} (a_N^2 - h_N^2) . \tag{2.33}$$

If a limit of this procedure when $N \rightarrow \infty$ exists, the resulting limiting matrices for large N provide a solution to the renormalization problem for the initial Hamiltonian H. It is visible that the unitarity constraints on the similarity matrix are satisfied only in the limit $N \rightarrow \infty$. Equation (2.33) implies unitarity constraints if $h_{N+1} \sim h_N$. One has to verify this procedure on a case by case basis, since it is not possible to generally determine if it is convergent. When the unitarity condition is satisfied the Hamiltonian H' is Hermitian and has the same spectrum as H.

Although H' does not introduce cutoff dependence to a desired order of perturbation theory for a sufficiently large Λ it may still happen that H' has large off-diagonal matrix elements so that its eigenstates may depend on the cutoff Λ in a genuinely nonperturbative way. An example of such situation is considered in Appendix B.

The bare Hamiltonian may be cut off in various ways, not necessarily only by restricting its domain. One may consider the initial Hamiltonian to have built in diagonal proximity bounds with $E_0 \sim \Lambda$ and/or β very large in comparison to 1. Then, one can reduce the bounds to finite E_0 and β in the same renormalization scheme. The resulting Hamiltonians H' for different parameters E_0 and β are related by a new renormalization-group relation.

We proceed to explain how the similarity method works in a model.

III. MODEL APPLICATION

In this section we present application of the similarity renormalization scheme to the model from Appendix B 1 of Ref. [5]. Our interest in the model was stimulated by a special case of the two-fermion bound-state eigenvalue problem in light-front quantum field theory. The model is exactly solvable and provides a well-understood testing ground.

The eigenvalue problem of the model is given in a form of the equation

$$(z+m)\phi(z) - g \int_0^\infty dz' \phi(z') = M \phi(z) . \qquad (3.1)$$

Originally, z denoted the square of the relative transverse momentum of two fermions, m was the square of the fermion mass, and g was the square of the fermion-boson coupling constant multiplied by the appropriate factors emerging in a one boson exchange effective interaction. M was the eigenvalue, equal to the mass squared of the corresponding eigenstate. $\phi(z)$ was a wave function describing the relative motion of fermions. In the present consideration those facts are mentioned merely for providing connection between the model and its origin [4,5]. The original Hamiltonian eigenvalue equation in quantum field theory involved complicated dynamics in a longitudinal direction. All these complications, including spin degrees of freedom, are removed here for simplicity.

The important feature of the eigenvalue problem in Eq. (3.1) is that the integral extends to infinity and generates divergences in the spectrum. An easy way to see a divergence is to notice that the wave function $\phi(z)$ falls off asymptotically as z^{-1} and the integral is logarithmically divergent. Renormalization of this model using differential equations in the effective Hamiltonian renormalization scheme is explained in Ref. [5]. Now, we shall test the similarity renormalization scheme armed with that experience.

We introduce the Hamiltonian H_0 and its eigenstates,

$$H_0|z\rangle = (z+m)|z\rangle , \qquad (3.2)$$

and the bare interaction V with the matrix elements

$$\langle z | V | z' \rangle = -g \quad . \tag{3.3}$$

Thus, our eigenvalue problem takes the form

$$(H_0 + V)|\phi\rangle = M|\phi\rangle . \tag{3.4}$$

It is convenient to denote matrix elements of all operators as functions of two arguments. For example,

$$\langle z|H_0|z'\rangle = H_0(z,z') = h_0(z)\delta(z-z')$$
, (3.5)

where $h_0(z) = z + m$, or

$$\langle z | \mathbf{DP}[V] | z' \rangle = \theta_P(z, z') V(z, z') , \qquad (3.6)$$

where $V(z,z') = \langle z | V | z' \rangle$ and $\theta_P(z,z')$ is a diagonal proximum factor. The latter is defined as

$$\theta_{P}(z,z') = \theta \left[\frac{\beta - 1}{\beta + 1} (E_{z} + E_{z'}) + \frac{2E_{0}}{\beta + 1} - |E_{z} - E_{z'}| \right],$$
(3.7)

where, according to Eq. (2.8), $E_z = z + m$, $E_{z'} = z' + m$, E_0 is a finite energy constant, and θ is the step function. The precise value of E_0 is not important. β must be greater than 1. The corresponding diagonal remotum factor is

$$\theta_R(z,z') = 1 - \theta_P(z,z') . \tag{3.8}$$

For example, the above definitions imply that $\theta_P(z,z')=1$ when

$$\beta z' + b > z > \frac{z' - b}{\beta} , \qquad (3.9)$$

where

$$b = \frac{\beta - 1}{2}c \tag{3.10}$$

and

$$c = 2\left[m + \frac{E_0}{\beta - 1}\right].$$
(3.11)

Thus, $\theta_R(z,z') = 1$ when

$$E_z - E_{z'} = |z - z'| \ge \frac{1}{B}(z + z' + c)$$
, (3.12)

where

$$B = \frac{\beta + 1}{\beta - 1} \tag{3.13}$$

Equation (3.12) is important, since it implies that the energy differences in denominators of perturbation theory are on the order of the energies themselves. Therefore, one is able to make estimates in perturbation theory without encountering problems with small denominators.

We consider expressions for operators V, Q, V', a, and h order by order in the coupling constant g. We need to explicitly discuss some features of Q up to third order in g in order to discover the structure of divergences and observe cancellations which occur in the similarity matrix T or its Hermitian conjugate. Then, the induction to all orders in g is explained.

We begin with first-order terms. From Eq. (2.22) we find that

$$Q_1(z,z') = V_1(z,z') = -1$$
. (3.14)

Consequently, from Eq. (2.23),

$$V_1'(z,z') = -\theta_P(z,z') , \qquad (3.15)$$

and from Eq. (2.24), we obtain that

$$a_1(z,z') = \frac{\theta_R(z,z')}{z-z'} .$$
 (3.16)

No divergence appears in the first order and there is no first order counterterm. In higher-order terms we need estimates on various first-order quantities. For example,

$$|Q_1(z,z')| \le c_1 , (3.17)$$

where c_1 is a finite positive constant. From Eqs. (3.12) and (3.16) it follows that

$$|a_1(z,z')| \le \frac{c_1}{z+z'+d_1}$$
, (3.18)

where this time $c_1 = B$ and $d_1 = c$. Similar estimates for higher-order terms involve powers of logarithms of z + z' + c.

5868

Our convention for using constants as c_1 and d_1 is following. When we consider estimates at certain order, for example, n, and derive a new bound which contains a constant, for example c_n , which is similar to a constant denoted earlier by the same symbol c_n in the already found bounds in this order, we replace the previous constant everywhere in the *n*th-order bounds by the new constant if the new constant gives bigger bounds. Thus, c_1 is a supremum of the sufficiently large constants from various bounds in first-order operators, and d_1 is an infimum of the sufficiently small constants. We use this convention in higher orders. We do not need to write the constants explicitly. We only need to know that such finite constants exist, since we do not yet consider the convergence of the series expansions in g. The convergence issue in this model is settled later.

The second-order term in Eq. (2.22) reads

$$Q_2 = V_2 - \{H_0, h_2\} + V_1' a_1 - a_1 V_1' + a_1 H_0 a_1 \quad (3.19)$$

From Eq. (2.20) we have $h_2 = \frac{1}{2}a_1^2$ and

$$h_{2}(z,z') = \frac{1}{2} \int_{0}^{\Lambda} dy \frac{\theta_{R}(z,y)}{z-y} \frac{\theta_{R}(y,z')}{y-z'} .$$
(3.20)

The integral for h_2 is convergent and $\{H_0, h_2\}$ is not sensitive to the cutoff. Terms involving V'_1 are finite thanks to the diagonal proximity condition on the transformed Hamiltonian, since the integration variables cannot reach the cutoff for finite arguments of $Q_2(z,z')$. The fifth term on the right-hand side (RHS) of Eq. (3.19) produces a divergence. Therefore, the counterterm V_2 is introduced. V_2 is defined by the condition that it removes the big Λ dependence from the fifth term. We need to find a form of the divergence and discover the corresponding structure of V_2 . Using Eqs. (3.5) and (3.16), we write

$$a_1 H_0 a_1(z,z') = \int_0^{\Lambda} dy \frac{\theta_R(z,y)}{z-y} (y+m) \frac{\theta_R(y,z')}{y-z'} . \quad (3.21)$$

For sufficiently large y the θ functions equal 1 and it is visible that there is a logarithmic divergence independent of z and z'. Therefore, the counterterm must be independent of z and z' also:

$$V_2(z,z') = v_2$$
 (3.22)

In order to cancel the logarithmic Λ dependence the constant v_2 must be of the form

$$v_2 = \ln \frac{\Lambda}{x_0} , \qquad (3.23)$$

where x_0 is an arbitrary finite scale. A useful way of writing v_2 is

$$v_2 = f_2 - \langle 0 | a_1 H_0 a_1 | 0 \rangle , \qquad (3.24)$$

where f_2 denotes an arbitrary finite constant and the second term cancels the logarithmic divergence in the fifth term. Thus, we obtain a conclusion that the z- and z'-independent counterterm V_2 , defined by Eqs. (3.22) and (3.24), removes the big Λ dependence from Q_2 . Evaluation of the integrals establishes that

$$Q_2(z,z') | \le c_2 \ln \frac{z+z'+c}{d_2}$$
, (3.25)

where c_2 and d_2 are some suitable positive constants. Equation (3.25) implies a similar bound on V'_2 , since $V'_2 = DP[Q_2]$. Moreover, for illustration, since

$$a_{2}(z,z') = \frac{\theta_{R}(z,z')}{z'-z} Q_{2}(z,z') , \qquad (3.26)$$

and the energy difference in the denominator is bounded from below by the diagonal remotum condition, we have a useful bound of the type

$$|a_2(z,z')| \le \frac{c_2}{z+z'+d_2} \ln \frac{z+z'+c}{d_2}$$
, (3.27)

which can be used in perturbative analysis to all orders in g (see Appendix A).

The third-order term in Q involves features which need to be discussed. From Eq. (2.22),

$$Q_{3} = V_{3} - \{H_{0}, h_{3}\} + V_{1}'(a_{2} - h_{2}) - (a_{2} + h_{2})V_{1}' + V_{2}'a_{1}$$

- $a_{1}V_{2}' + a_{1}H_{0}(a_{2} - h_{2}) + (a_{2} + h_{2})H_{0}a_{1} + a_{1}V_{1}'a_{1}$.
(3.28)

Terms involving products of three operators are divergent. For example, consider the term $-a_1H_0h_2$. The divergence originates from the region where H_0 in the intermediate state is order Λ . From Eq. (3.20) one can see that $h_2(y,z')$ for $y \sim \Lambda$ contains terms of the form

$$\frac{1}{2y}\ln\left[\frac{z'}{b} + \frac{1}{\beta - 1}\right]$$
(3.29)

and such term leads to a logarithmic divergence in $\langle z|-a_1H_0h_2|z'\rangle$ which is multiplied by the logarithmic function of z'. However, this z' dependent divergence is canceled when one adds the term $a_1H_0a_2$. This is a generic cancellation. It occurs in the matrix elements

$$-T^{\dagger}(y,z') = \langle y | (a-h) | z' \rangle$$

when the left y is much larger than the right z' and in

$$T(z,y) = \langle z | (a+h) | y \rangle$$

when the right y is much bigger than the left z. For example, consider the matrix element

$$\langle y|(a_2-h_2)|z'\rangle = \frac{1}{h_0(y)} \langle y|H_0(a_2-h_2)|z'\rangle$$
 (3.30)

Using Eqs. (2.13) and (2.15),

$$H_0(a_2 - h_2) = -\mathbf{DR}[Q_2] - \{H_0, h_2\} + (h_2 + a_2)H_0 \quad (3.31)$$

and for sufficiently large y the diagonal remotum factor $\theta_R(y,z')$ equals 1, so that the matrix element of $DR[Q_2]$ equals the matrix element of Q_2 itself. Then,

$$\langle y|H_{0}(a_{2}-h_{2})|z'\rangle = \langle y|[-V_{2}-V_{1}'a_{1}+a_{1}V_{1}'-a_{1}H_{0}a_{1} + (a_{2}+h_{2})H_{0}]|z'\rangle .$$
(3.32)

An examination of this formula shows that $a_2 - h_2$ no longer contains any z' dependence in order 1/y, despite such a term in h_2 . One can compare the matrix element in Eq. (3.32) with

$$\langle y | H_0(a_2 - h_2) | 0 \rangle$$

and see that the difference is order y^{-1} , so that the matrix element in Eq. (3.30) does not contain a z'-dependent term order y^{-1} , since the inverse of $h_0(y)$ provides another factor of y^{-1} and the divergence in

$$\langle z|a_1H_0(a_2-h_2)|z'\rangle$$

is independent of z'. These cancellations suggest that we should consider matrices a and h together, in the sums and differences. It is convenient to consider a and h without separating them despite that h is expressed by a through Eqs. (2.5) or (2.20), since it helps to see that the divergences are independent of the external states' energies, i.e., independent of z and z'. Thus,

$$V_3(z,z') = v_3$$
, (3.33)

where

$$v_{3} = f_{3} - \langle 0 | [a_{1}H_{0}(a_{2}-h_{2}) + (a_{2}+h_{2})H_{0}a_{1} + a_{1}V_{1}a_{1}] | 0 \rangle , \qquad (3.34)$$

in analogy to Eqs. (3.22) to (3.24). A comment is in order about the last term. Terms of such structure do not appear in Q_1 and Q_2 . The last term is divergent because there are two intermediate variables to integrate over, for example, x and y. Although the two variables have to be close to each other according to the diagonal proximum condition on V'_1 , the width of $\theta_P(x,y)$ grows with x + y. Therefore, this term is logarithmically divergent, since $a_1(z,x)$ and $a_1(y,z')$ fall off as only one inverse power of a big argument. However, the counterterm V_3 , in particular its part $-\langle 0|a_1V'_1a_1|0\rangle$, removes the divergence. As a result,

$$|Q_{3}(z,z')| \le c_{3} \ln^{2} \frac{z+z'+c}{d_{3}}$$
(3.35)

and also

$$|a_3(z,z')| \le \frac{c_3}{z+z'+d_3} \ln^2 \frac{z+z'+c}{d_3}$$
 (3.36)

Equations (3.24) and (3.34) suggest a general method of estimating matrix elements of subtracted operators,

which we have also adopted in Ref. [5]. Namely, the counterterms remove Λ dependence from matrix elements of an operator \hat{O} and produce finite matrix elements of a new subtracted operator \hat{o} in the following generic way:

$$\langle z|\hat{o}|z'\rangle = \langle z|\hat{O}|z'\rangle + o_f - \langle 0|\hat{O}|0\rangle , \qquad (3.37)$$

where o_f denotes an arbitrary finite part. Equation (3.37) can be rewritten as

$$\langle z|\hat{o} |z'\rangle = o_f + (\langle z| - \langle 0|)\hat{O} |z'\rangle$$

+ $\langle 0|\hat{O}(|z'\rangle - |0\rangle) .$ (3.38)

Therefore, it is useful to consider bounds on the differences of matrix elements of the type appearing on the RHS of Eq. (3.38), and use these bounds in proving finiteness of subtracted operators in the limit $\Lambda \rightarrow \infty$.

At this point it is demonstrated that constant counterterms of second and third order remove divergences from Q_2 and Q_3 , respectively. Q_1 is given by the bare interaction and contains no counterterm. A proof by mathematical induction that the constant counterterms remove the big cutoff dependence from the "band-diagonal" Hamiltonian matrix elements to all orders in the coupling constant g is sketched in Appendix A.

IV. CONCLUSION

It is recursively established for all powers of the coupling constant g that a constant counterterm is sufficient to remove the cutoff dependence from the matrix elements of the Hamiltonian H' for finite indices. Therefore, one can always make the cutoff Λ big enough so that all terms in perturbation theory up to an arbitrary order p are independent of the cutoff. Suppose we consider correction to a state of a free energy E. Then, using the diagonal proximum condition from Eq. (3.9), we see that for large Λ the new interaction Hamiltonian V' cannot reach the cutoff until sufficiently high-order terms of perturbation expansions are considered. For example, no cutoff dependence appears up to the order g^{2p} when $\Lambda \ge x_p(E)$, where the function x_p is explained in Eqs. (A9) and (A10) in Appendix A. Thus, making the cutoff Λ infinitely large removes the cutoff dependence from the eigenvalue problem of the Hamiltonian H to all orders of the perturbation theory.

One possible way of proceeding further is to try to construct the effective Hamiltonian H' in the iteration procedure described in Eqs. (2.26) to (2.33), and solve this Hamiltonian with a sufficiently large cutoff Λ . The counterterm V_{N+1} is defined through its matrix elements:

$$\langle z|V_{N+1}|z'\rangle = f_{N+1} - \langle 0|[-\{H_0, h_N\} + H'_{IN}(a_N - h_N) - (a_N + h_N)H'_{IN} + (a_N + h_N)H'_N(a_N - h_N)]|0\rangle , \qquad (4.1)$$

Various choices of E_0 and β in the definition of the diagonal proximum lead to corresponding Hamiltonians with various widths and slopes of their "band-diagonal" structure. These Hamiltonians are related by a new kind of renormalization-group transformation which is

parametrized by E_0 and β . It is interesting to note that the diagonal proximum structure of the effective renormalized Hamiltonian resembles to some extent phenomenologically useful vertex form factors which limit allowed momentum and/or energy transfers in acts of emission or absorption of particles.

One can also proceed in a more direct way without constructing the "band-diagonal" Hamiltonians. Namely, one can write the Hamiltonian H which contains an arbitrary counterterm constant v in its kernel in addition to the coupling constant g. Then, one can solve the eigenvalue problem for the Hamiltonian H, calculate some low energy observable and try to vary the big Λ . One may observe that when Λ is sufficiently large, it is enough to keep changing the constant v together with changing Λ in order to always obtain a fixed value of the chosen observable, independently of Λ . This way one generates a function v of Λ . The arbitrary magnitude of the constant v can be fixed by requesting a definite value of the chosen observable for some value of the cutoff, $\Lambda = \Lambda_0$.

This conclusion can be verified by analytic calculations. The result, given in Ref. [5], Eq. (B4), is

$$v(\Lambda) = \frac{f - g(f + g) \ln \Lambda / \Lambda_0}{1 + (f + g) \ln \Lambda / \Lambda_0} , \qquad (4.2)$$

where $f = v(\Lambda_0)$ is an arbitrary finite constant to be fixed by the preferred value for the chosen observable. With this choice for the function $v(\Lambda)$ all observables become independent of Λ when $\Lambda \rightarrow \infty$. At this point we have also settled the convergence issue in the model, since the series expansion from Eq. (2.16) sums up to the result in Eq. (4.2). Namely,

$$\langle z|V|z'\rangle = -g - v(\Lambda)$$
 (4.3)

The simplified test model is solvable analytically and contains only one free parameter which needs to be adjusted when the cutoff is changed. In more complicated models the situation is different and there is little hope that adjusting a single parameter somewhere in a Hamiltonian removes cutoff dependence from its eigenvalue problem. The similarity renormalization scheme helps in finding the structure of required counterterms and deciding what is allowed to depend on the cutoff. One tries to construct or fit the cutoff dependence of the counterterms so that the resulting observables are independent of the cutoff. The cutoff independence hinges on the accuracy of a procedure.

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APPENDIX A

It is explained in Sec. III that constant counterterms of second and third order remove divergences from Q_2 and Q_3 , respectively. Q_1 is given by the bare interaction and contains no counterterm. In this Appendix we sketch a proof for that knowing N-1 constant counterterms V_2 , V_3, \ldots, V_{N-1} , and V_N , which make matrix elements of $Q_2, Q_3, \ldots, Q_{N-1}$, and Q_N with finite indices become independent of the big cutoff $\Lambda \rightarrow \infty$, respectively, one can define the next order counterterm, V_{N+1} , which is also constant and makes the matrix elements of Q_{N+1} with finite indices become independent of the big cutoff in the big cutoff

the limit $\Lambda \rightarrow \infty$.

Following the analysis of low order terms, we write Q_n , for n = 1, 2, 3, ..., N as

$$Q_{n} = V_{n} - \{H_{0}, h_{n}\} + \sum_{i=1}^{n-1} V_{i}' r_{n-i} - \sum_{i=1}^{n-1} l_{n-i} V_{i}' + \sum_{i=1}^{n-1} l_{i} H_{0} r_{n-i} + \sum_{i=1}^{n-2} \sum_{j=1}^{n-1-i} l_{i} V_{j}' r_{n-i-j}, \qquad (A1)$$

where $l_i = a_i + h_i$ and $r_i = a_i - h_i$ for all *i*. The counterterms V_n for n = 2, 3, ..., N have the matrix elements

$$\langle z|V_n|z'\rangle = v_n$$
, (A2)

where the constants v_n are

$$v_{n} = f_{n} - \sum_{i=1}^{n-1} \langle 0 | l_{i} H_{0} r_{n-i} | 0 \rangle + \sum_{i=1}^{n-2} \sum_{j=1}^{n-1-i} \langle 0 | l_{i} V_{j}' r_{n-i-j} | 0 \rangle , \qquad (A3)$$

and f_n are arbitrary finite numbers.

The following bounds are assumed to be valid for matrix elements of various operators for n = 1, 2, ..., N in the limit $\Lambda \rightarrow \infty$:

$$|Q_n(z,z')| \le c_n \ln^{n-1} \frac{z+z'+c}{d_n}$$
, (A4)

$$|l_n(z,z')| \le \frac{c_n}{z+z'+d_n} \ln^{n-1} \frac{z+z'+c}{d_n}$$
, (A5)

$$|r_n(z,z')| \le \frac{c_n}{z+z'+d_n} \ln^{n-1} \frac{z+z'+c}{d_n}$$
, (A6)

$$|l_n(z,y) - l_n(0,y)| \le \frac{c_n}{y} \frac{h_0(z)}{h_0(y)} \ln^{n-1} \frac{z+y+c}{d_n}$$
(A7)

for $y \ge x_n(z)$, and

$$|r_n(y,z') - r_n(y,0)| \le \frac{c_n}{y} \frac{h_0(z')}{h_0(y)} \ln^{n-1} \frac{y+z'+c}{d_n}$$
(A8)

for $y \ge x_n(z')$, where

$$x_n(z) = x_1[x_{n-1}(z)]$$
 (A9)

and

$$x_1(z) = \beta z + b \quad . \tag{A10}$$

The above bounds imply that we also assume that

$$|h_{N+1}(z,z')| \le \frac{c_{N+1}}{z+z'+d_{N+1}} \ln^N \frac{z+z'+c}{d_{N+1}}$$
 (A11)

Then, we define Q_{N+1} :

$$Q_{N+1} = V_{N+1} - \{H_0, h_{N+1}\} + \sum_{i=1}^{N} V'_i r_{N+1-i}$$
$$- \sum_{i=1}^{N} l_{N+1-i} V'_i + \sum_{i=1}^{N} l_i H_0 r_{N+1-i}$$
$$+ \sum_{i=1}^{N-1} \sum_{j=1}^{N-i} l_i V'_j r_{N+1-i-j} .$$
(A12)

Matrix elements of the counterterm V_{N+1} are

$$\langle z|V_{N+1}|z'\rangle = v_{N+1} , \qquad (A13)$$

and the constant v_{N+1} is

$$v_{N+1} = f_{N+1} - \sum_{i=1}^{N} \langle 0 | l_i H_0 r_{N+1-i} | 0 \rangle + \sum_{i=1}^{N-1} \sum_{j=1}^{N-i} \langle 0 | l_i V'_j r_{N+1-i-j} | 0 \rangle .$$
 (A14)

 f_{N+1} is an arbitrary finite number.

One can follow discussion of Eqs. (3.30)-(3.32) in Sec. III and show that the bounds from Eqs. (A4) to (A11) and the above definition of the counterterm V_{N+1} imply the following bounds on matrix elements of various operators of the order g^{N+1} in the limit $\Lambda \rightarrow \infty$:

$$|Q_{N+1}(z,z')| \le c_{N+1} \ln^N \frac{z+z'+c}{d_{N+1}}$$
, (A15)

$$|l_{N+1}(z,z')| \le \frac{c_{N+1}}{z+z'+d_{N+1}} \ln^{N} \frac{z+z'+c}{d_{N+1}}$$
, (A16)

$$|r_{N+1}(z,z')| \le \frac{c_{N+1}}{z+z'+d_{N+1}} \ln^{N} \frac{z+z'+c}{d_{N+1}}$$
, (A17)

$$|l_{N+1}(z,y) - l_{N+1}(0,y)| \le \frac{c_{N+1}}{y} \frac{h_0(z)}{h_0(y)} \ln^N \frac{z+y+c}{d_{N+1}}$$
(A18)

for $y \ge x_{N+1}(z)$, and

$$|r_{N+1}(y,z') - r_{N+1}(y,0)| \le \frac{c_{N+1}}{y} \frac{h_0(z')}{h_0(y)} \ln^N \frac{y+z'+c}{d_{N+1}}$$
(A19)

for $y \ge x_{N+1}(z')$, where

$$x_{N+1}(z) = x_1[x_N(z)]$$
 (A20)

These bounds imply that

$$|h_{N+2}(z,z')| \le \frac{c_{N+2}}{z+z'+d_{N+2}} \ln^{N+1} \frac{z+z'+c}{d_{N+2}}$$
 (A21)

Thus, by mathematical induction, we know that a constant counterterm can remove the cutoff dependence from the matrix elements of Q to all orders in the coupling constant g. Therefore, it also removes the cutoff dependence from the Hamiltonian H' to all orders in g, since the cutoff independence of the matrix elements of Q implies the cutoff independence for the matrix elements with finite indices of the new interaction Hamiltonian, V' = DP[Q].

APPENDIX B

This appendix contains an example of a "banddiagonal" Hamiltonian which exhibits nonperturbative cutoff dependence due to large off-diagonal matrix elements. The $N \times N$ Hamiltonian matrix is

$$H = \begin{bmatrix} \omega & a \\ a & \lambda \omega & \lambda a \\ & \lambda a & \lambda^2 \omega & \lambda^2 a \\ & & \lambda^2 a & \lambda^3 \omega & \ddots \end{bmatrix}, \quad (B1)$$

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and its eigenvector is

r

$$\Psi = \begin{vmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{vmatrix} . \tag{B2}$$

The eigenvalue equations are

$$E\psi_n = \lambda^{n-1}a\psi_{n-1} + \lambda^n \omega \psi_n + \lambda^n a\psi_{n+1} .$$
 (B3)

Solving these equations by elimination starting with ψ_N and denoting

$$\psi_n = \gamma_n \psi_{n-1} , \qquad (B4)$$

one has

$$\gamma_n = \frac{\lambda^{n-1}a}{E - \lambda^n \omega - \lambda^n a \gamma_{n+1}}$$
(B5)

and $\gamma_{N+1}=0$. If E is bounded and n is large with $\lambda > 1$ then

$$\gamma_n \simeq -\frac{a}{\lambda} \frac{1}{\omega + a\gamma_{n+1}} . \tag{B6}$$

One can make a plot which shows how γ_n depends on γ_{n+1} , which is a hyperbola with its vertical asymptote at $\gamma_{n+1} = -\omega/a$. One can use this plot to show that if the fixed points γ^* ,

$$\gamma^* = -\frac{a}{\lambda} \frac{1}{\omega + a\gamma^*} , \qquad (B7)$$

are real then the smaller of the two is stable and all sequences γ_n converge to this stable fixed point unless one starts at the unstable point. If *a* is large enough the fixed points are complex and all sequences cycle chaotically forever.

If the sequence of γ_n 's converges then the eigenvalue equation has a limit for $N \rightarrow \infty$ as predicted by perturbation theory. The opposite case corresponds to the situation when the matrix H has large negative eigenvalues which is undesirable for other reasons. This could imply only that new counterterms are needed for the theory to make sense, including an overall energy shift to bring the lowest energy to be at order 1 instead of large.

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