PHYSICAL REVIEW D VOLUME 19, NUMBER 8 15 APRIL 1979

# Improved strong-coupling expansions and matrix Padé approximants for lattice theories

Allen Carroll*
*Centre d'Etudes Nucleaires, Saclay, B.P. N°2, F-91190 Gif-sur-Yvette, France*

John B. Kogut
*Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*
(Received 22 November 1978)

A generalization of Hamiltonian perturbation theory is presented. The method solves a low-energy sector of the theory exactly while systematically accounting for higher-energy states perturbatively. It produces an expansion for the mass matrix of the low-energy sector. In applications to lattice theories, the mass matrix can be extrapolated to the continuum limit using matrix Padé approximants. The method is illustrated for a lattice potential model and fast convergence to the continuum limit is verified numerically.

## I. INTRODUCTION

Hamiltonian strong-coupling expansions[1] provide one with a systematic calculational program for dealing with strong-coupling problems in discrete-spin systems and lattice gauge theory. The method has had some success, using extrapolation procedures such as Padé approximants, for finding approximate results in continuum field theories which are weakly coupled at short distances. Strong-coupling expansions have been applied to spin systems to determine phase diagrams[2] and to model field theories to study spontaneous mass generation,[3] quark confinement,[4] mass spectra,[5] and continuum limits. The method's most grandiose aim is the calculation of the mass spectrum of quantum chromodynamics in 3+1 dimensions. Even for this theory, low-order results are in many cases quite reasonable.[6] The following mass ratios are a sample of results:

$$m_\rho/m_N = 0.822 \quad (0.820),$$
$$m_\omega/m_N = 0.824 \quad (0.834),$$
$$m_\pi/m_N = 0.820 \quad (0.147),$$
$$m_\sigma/m_N = 0.972 \quad (1.0, \text{broad}),$$
$$m_B/m_N = 1.05 \quad (1.32),$$
$$m_f/m_N = 1.17 \quad (1.35),$$
$$m_{A_1}/m_N = 1.12 \quad (1.17),$$
$$f_\pi m_\rho/f_\rho = 0.7 \quad (0.70),$$

where the numbers in parentheses are the experimental values for these ratios. It is interesting that these predictions involve no free parameters. The lattice coupling $g$ does not appear in the mass ratio because $g$ vanishes in the continuum limit as a consequence of asymptotic freedom. We see from this list that all the mass ratios are calculated quite well except for the pion. The pion should, in fact, be massless in quantum chromodynamics formulated with an isodoublet of massless quarks if the ground state spontaneously breaks chiral SU(2) symmetry.[1] Unfortunately, this symmetry is broken by the lattice fermion method used to represent quark fields in Ref. 6 so although the continuous symmetry is expected to emerge in the continuum limit of the lattice theory, these calculations are not sufficiently accurate (of high enough order) to establish this.

Other strong-coupling calculations of the mass spectrum have been performed using different lattice fermion methods. In those which do not explicitly break chiral SU(2) symmetry, a massless pion is naturally obtained. However, then low-order calculations do not produce realistic nucleon-$\Delta$ splittings or a sufficiently massive $\eta$. Clearly, better calculational techniques are needed as well as higher-order expansions. It seems particularly important to attack the difficult features of the mass spectrum with accuracy and not be satisfied with rough estimates of the masses of many states. In this regard the nucleon-$\Delta$ and the $\pi$-$\eta$ splittings are important quantities. To appreciate this recall that in the MIT bag model[7] the $s$-wave pseudoscalar mesons required the calculation of instanton effects within each hadron to explain how the pion could be so light while the $\eta$ could be so heavy.[8] And the nucleon-$\Delta$ splitting required relatively hard gluon exchange between the quark constituents of these baryons. If these explanations are correct physically, lattice calculations, which begin with a strongly coupled version of the theory on a coarse lattice, will be severely challenged to obtain accurate numbers.

In this article a rather elaborate strong-coupling method will be introduced and illustrated. It is a straightforward generalization of strong-coupling expansions.[5] It can also yield approximate continuum-limit results. The idea of the method is as

 

follows. In an ordinary perturbation theory approach one writes the Hamiltonian as the sum of two pieces, $H=H_0+\lambda V$. The "large" term $H_0$ is presumably solvable and one has its spectrum $\{\epsilon_a, |a\rangle\}$ of eigenvalues and eigenvectors. The eigenvectors of $H$ will, in simple cases, be in one-to-one correspondence with those of $H_0$ and expansions for the spectrum $\{E_a, |A\rangle\}$ of $H$ in terms of the spectrum for $H_0$ can be obtained,

$$E_a=\epsilon_a+\sum_{n=1}^{\infty}\lambda^n c_n,$$
$$|A\rangle=|a\rangle+\sum_{n=1}^{\infty}\lambda^n\sum_{i\neq a}b_{ni}|i\rangle. \tag{1.1}$$

Raleigh-Schrödinger perturbation theory gives explicit formulas for the coefficients $c_n$ and $b_{ni}$ in terms of matrix elements of the perturbation $V$ in the known spectrum of $H_0$. In the case that the state $|a\rangle$ is degenerate with other eigenstates of $H_0$, these formulas must and can be modified in a simple way. The type of perturbation theory to be developed here will generalize these familiar cases. Its aim is to solve the "low"-energy sector of $H$. The method will account for the interactions and mixing among the states of the low-energy sector *exactly* while accounting for the influence of the high-energy states upon the low-energy sector perturbatively. In so doing, we can hope to obtain a more accurate determination of the properties of the low-energy sector of the theory than is done in ordinary perturbation theory where *all* effects of $V$ are treated perturbatively. Clearly this approach is a type of "momentum slicing" and has much in common with renormalization-group calculations.

In summary, we will split the spectrum of $H_0$ into a low-energy subspace $S_L$ and a high-energy subspace $S_H$. The Hamiltonian will be diagonalized exactly within $S_L$ and the effect of $S_H$ on $S_L$ will be computed perturbatively. Formulas correct to all orders in $\lambda$ are needed and will be recorded in the text. In practice one chooses $S_L$ to be rather small but still elaborate enough so that good estimates for the low-energy spectrum of $H$ can be obtained without needing to do many terms in the strong-coupling expansion. Of course, the mass of a particle of $H$ should be independent of the exact size of $S_L$.

As one would expect this perturbation theory is not new. It has been used in atomic and nuclear physics where it is referred to as an "effective operator" method.[9,10] We will develop it in an elementary fashion in the text because it is not familiar to many physicists outside of these specialties. However, the more technical aspects of the method—such as a proof that a connected formalism exists[9]—will be left to the references. This article, however, will provide all the formulas needed to employ the method and the statements that the method makes sense (for example, that particle masses are intensive quantities).

After the perturbation theory for a lattice Hamiltonian has been set down, we need a method of taking the continuum limit. In past calculations, dimensionless quantities such as mass ratios and matrix elements were extrapolated to the continuum limit using diagonal Padé approximants. Since diagonal Padé approximants possess nontrivial invariance properties and are known to converge for a wide class of functions, this extrapolation method has been used with success in many calculations of atomic, statistical, and mathematical physics. In the scheme here, we need to extrapolate a mass *matrix* for the subspace $S_L$. A natural way to do this is with matrix Padé approximants.[11,12] Matrix approximants are discussed in the text and their mathematical properties which suggest that they are a good way to use our perturbation theory expansions are reviewed.

Finally, we will present an example of the technique. We will compute the first few levels of the lattice linear potential model and note that the method produces levels which appear to converge quickly to the correct continuum values. This example is simple enough that it will be clear why these matrix methods can produce better series than the simplest, one-state, strong-coupling expansions. A discussion of other calculations in progress constitutes our concluding remarks.

## II. MATRIX BRILLOUIN-WIGNER PERTURBATION THEORY

Suppose we wish to solve the Hamiltonian

$$H=H_0+\lambda V \tag{2.1}$$

given the spectrum of $H_0$. Separate the spectrum of $H_0$ into a "low"-energy part and a "high"-energy part,

$$\{\epsilon_i, |\phi_i\rangle\}\text{: "low" energy},\qquad \{\epsilon'_J, |\phi'_J\rangle\}\text{: "high" energy}. \tag{2.2}$$

Our problem is the computation of the low-energy spectrum of $H$,

$$H|\psi_j\rangle=E_j|\psi_j\rangle, \tag{2.3}$$

in which the "low"-energy states $\{|\phi_i\rangle\}$ are treated exactly and the "high"-energy states $\{|\phi'_J\rangle\}$ are treated perturbatively. First we obtain an implicit matrix equation for $E_j$ by generalizing the method of Brillouin and Wigner.[13]

Since the spectrum of $H_0$ is assumed to be complete we can write

$$|\psi_j\rangle=\sum_k |\phi_k\rangle\langle\phi_k|\psi_j\rangle+\sum_J |\phi'_J\rangle\langle\phi'_J|\psi_j\rangle. \quad (2.4)$$

This will be a useful formula if the amplitudes $\langle\phi'_J|\psi_j\rangle$ can be computed in a power series in $\lambda$. To do this, project Eq. (2.3) against the state $|\phi'_J\rangle$,

$$\langle\phi'_J|H-H_0|\psi_j\rangle=\lambda\langle\phi'_J|V|\psi_j\rangle, \quad (2.5a)$$

which gives

$$\langle\phi'_J|\psi_j\rangle=\frac{\lambda}{E_j-\epsilon'_J}\langle\phi'_J|V|\psi_j\rangle. \quad (2.5b)$$

To simplify the notation define

$$\langle\phi_i|\psi_j\rangle\equiv a_{ij}, \quad \langle\phi'_J|\psi_j\rangle\equiv a'_{Jj}. \quad (2.6)$$

Then if $H$ is applied to Eq. (2.4),

$$H|\psi_j\rangle=E_j|\psi_j\rangle=\sum_k(\epsilon_k+\lambda V)|\phi_k\rangle a_{kj} + \sum_J(\epsilon'_J+\lambda V)|\phi'_J\rangle a'_{Jj}. \quad (2.7)$$

Projecting this equation against $|\phi_i\rangle$,

$$E_j a_{ij}=\sum_k(\epsilon_k\delta_{ik}+\lambda V_{ik})a_{kj}+\sum_J\lambda V_{iJ}a'_{Jj}. \quad (2.8)$$

Using Eqs. (2.5b) and (2.8), our problem is solved. Substituting Eq. (2.5b) into the last term of Eq. (2.8) gives

$$E_j a_{ij}=\sum_k(\epsilon_k\delta_{ik}+\lambda V_{ik})a_{kj} + \sum_J\lambda V_{iJ}\frac{1}{E_j-\epsilon'_J}\lambda\langle\phi'_J|V|\psi_j\rangle, \quad (2.9)$$

which can be solved by iteration. In particular, iterate Eq. (2.5b) one step,

$$a'_{Jj}=\frac{\lambda}{E_j-\epsilon'_J}\langle\phi'_J|V|\psi_j\rangle =\frac{\lambda}{E_j-\epsilon'_J}\langle\phi'_J|V\Big(\sum_k|\phi_k\rangle\langle\phi_k| + \sum_{J'}|\phi'_{J'}\rangle\langle\phi'_{J'}|\Big)|\psi_j\rangle =\frac{\lambda}{E_j-\epsilon'_J}\Big(\sum_k V_{Jk}a_{kj}+\sum_{J'}V_{JJ'}a_{J'j}\Big). \quad (2.10)$$

Inserting this result into Eq. (2.8) gives

$$E_j a_{ij}=\sum_k\Big(\epsilon_k\delta_{ik}+\lambda V_{ik}+\sum_J\lambda V_{iJ}\frac{1}{E_j-\epsilon'_J}\lambda V_{Jk}\Big)a_{kj} + \sum_{J,J'}\lambda V_{iJ}\frac{1}{E_j-\epsilon'_J}\lambda V_{JJ'}a_{J'j}. \quad (2.11)$$

So, to determine $E_j$ to second order in $\lambda$, the last term in this equation can be dropped and the $E_j$ can be obtained self-consistently by diagonalizing the matrix in parentheses. If the low-energy subspace were one dimensional, then this result reduces to the more familiar Brillouin-Wigner perturbation expansion. If the low-energy subspace were degenerate in zeroth order, then the equation again reduces to another more familiar special case. By substituting Eq. (2.10) into Eq. (2.11) repeatedly, one finds,

$$E_j a_{ij}=\sum_k\Big(\epsilon_k\delta_{ik}+\lambda V_{ik}+\sum_{J_1}\lambda V_{iJ_1}\frac{1}{E_j-\epsilon'_{J_1}}\lambda V_{J_1k}+\cdots + \sum_{J_1,\ldots,J_N}\lambda V_{iJ_1}\frac{1}{E_j-\epsilon'_{J_1}}\lambda V_{J_1J_2}\frac{1}{E_j-\epsilon'_{J_2}}\lambda V_{J_2J_3}\cdots\lambda V_{J_Nk}\Big)a_{kj} + \sum_{J_1,\ldots,J_{N+1}}\lambda V_{iJ_1}\frac{1}{E_j-\epsilon'_{J_1}}\lambda V_{J_1J_2}\frac{1}{E_j-\epsilon'_{J_2}}\lambda V_{J_2J_3}\cdots\lambda V_{J_NJ_{N+1}}a'_{J_{N+1}j}. \quad (2.12)$$

So, to compute $E_j$ to $N$th order in $\lambda$, the last term in this equation can be dropped. Then Eq. (2.12) reduces to a matrix in the "low"-energy subspace. It is still an implicit equation for $E_j$ but it does treat the mixing within the low-energy subspace exactly while the influence of the high-energy states is accounted for systematically in perturbation theory. Later in this article Eq. (2.12) will be written in Raleigh-Schrödinger form as an *explicit* formula for the eigenvalues $E_j$.

It is best to rewrite Eq. (2.12) in a more abstract but clearer form. Define the projection

operator $P$ onto the low-energy subspace $S_L$ and let $Q=1-P$. Define a resolvent,

$$G(E)=\frac{Q}{E-H_0}. \tag{2.13}$$

Next let $\psi_j$ be the projection of the exact state $|\psi_j\rangle$ onto the low-energy subspace. In the notation of Eq. (2.12), $\psi_j$ is the column matrix

$$\psi_j=[a_{ij}]\,. \tag{2.14}$$

Now Eq. (2.12) can be written as a time-independent Schrödinger equation with an energy-dependent potential,

$$(E-\epsilon)\psi=\mathcal{V}(E)\psi\,, \tag{2.15}$$

where $\epsilon$ is the unperturbed energy matrix

$$\begin{bmatrix} \epsilon_1 & 0 & 0 & \cdots \\ 0 & \epsilon_2 & 0 & \\ 0 & 0 & \epsilon_3 & \\ \vdots & & & \ddots \end{bmatrix} \tag{2.16}$$

and the effective potential $\mathcal{V}(E)$ is

$$\mathcal{V}(E)=P[V+VG(E)V+VG(E)VG(E)V+\cdots]P\,, \tag{2.17}$$

where the projection operators $P$ remind us that Eq. (2.15) is a finite-dimensional matrix equation in the subspace $S_L$. Here $E$ is just a number which represents one of the eigenvalues $E_j$ of the implicit eigenvector-eigenvalue problem, Eq. (2.15).

## III. MATRIX RALEIGH-SCHRODINGER PERTURBATION THEORY

The "Schrödinger" equation in the low-energy subspace,

$$(E-\epsilon)\psi=\mathcal{V}(E)\psi\,, \tag{2.15}$$

can be used to determine the energies $E_j$ self-consistently. Alternatively, one can find an explicit formula for $E_j$ by generalizing the usual procedure of passing from a Brillouin-Wigner perturbation expansion to a Raleigh-Schrödinger expansion. We will do this exercise here for the case that $S_L$ is two dimensional. This choice is made for easy presentation—the generalization to larger subspaces is straightforward.

To begin, organize Eq. (2.15) so that it has the appearance of ordinary two-state *degenerate* Brillouin-Wigner perturbation theory. Let $\epsilon_a$ and $\epsilon_b$ ($\epsilon_a\neq\epsilon_b$) be the unperturbed energies of the states in $S_L$, but organize the Hamiltonian as

$$H=\hat{H}_0+\hat{V}\,, \tag{3.1a}$$

where

$$\hat{H}_0=H_0-\Delta P_b\,,\quad \hat{V}=\lambda V+\Delta P_b \tag{3.1b}$$

$$\Delta=\epsilon_b-\epsilon_a\,, \tag{3.1c}$$

and

$$P_a=\text{projection operator on } |\phi_a\rangle\,,$$
$$P_b=\text{projection operator on } |\phi_b\rangle\,. \tag{3.1d}$$

The value in writing Eq. (3.1a) is that $\hat{H}_0$ has the same value when applied to either $|\phi_a\rangle$ or $|\phi_b\rangle$,

$$\begin{aligned}\hat{H}_0|\phi_a\rangle&=\epsilon_a|\phi_a\rangle\,,\\ \hat{H}_0|\phi_b\rangle&=\epsilon_a|\phi_b\rangle\,.\end{aligned} \tag{3.2}$$

This fact will help in making the transition from Brillouin-Wigner to Raleigh-Schrödinger perturbation theory. The price one has paid is that $V$ contains the operator $\Delta P_b$ which is zeroth order in $\lambda$. However, this additional term has such a simple structure that for *any* given order in $\lambda$ it can be accounted for to *all* orders. So, in the end we shall have a conventional perturbation expansion in $\lambda$ and the levels $\epsilon_a$ and $\epsilon_b$ will be arbitrary.

For the decomposition of Eq. (3.1a), the effective potential has the form

$$\mathcal{V}(E)=\hat{V}+\hat{V}\frac{Q}{E-\hat{H}_0}\hat{V}+\hat{V}\frac{Q}{E-\hat{H}_0}\hat{V}\,\frac{Q}{E-H_0}\hat{V}+\cdots\,, \tag{3.3}$$

where $Q=1-P_a-P_b$ and the factors of $P=P_a+P_b$ which appear in Eq. (2.17) have not been written in explicitly. Since

$$QP_b=P_bQ=0\,, \tag{3.4}$$

we have

$$Q\hat{V}=QV\,,\quad \hat{V}Q=VQ \tag{3.5a}$$

and

$$\frac{Q}{E-\hat{H}_0}=\frac{Q}{E-H_0}. \tag{3.5b}$$

So, Eq. (3.3) simplifies to

$$\mathcal{V}(E)=\Delta P_b+V+VG(E)V+VG(E)VG(E)V+\cdots\,, \tag{3.6}$$

using Eq. (2.13). It is convenient to define two more resolvents,

$$g_a=\frac{Q}{\epsilon_a-H_0}\,,\quad g_b=\frac{Q}{\epsilon_b-H_0}. \tag{3.7}$$

Then

$$G(E)=\frac{Q}{E-H_0}=\frac{Q}{\epsilon_a-H_0-(\epsilon_a-E)}$$

$$=\sum_{n=0}^{\infty}\left(\frac{Q}{\epsilon_a-H_0}\right)^{n+1}(\epsilon_a-E)^n$$

$$=\sum_{n=0}^{\infty}g_a^{n+1}(\epsilon_a-E)^n. \tag{3.8}$$

Recall that $E$ denotes one of the eigenvalues $E_j$, so there is no problem with operator ordering in Eq. (3.8). If this expansion is substituted into Eq. (2.15) we have

$$(E-\epsilon_a)\psi=[\Delta P_b+V+VG(E)V+VG(E)VG(E)V+\cdots]\psi$$

$$=\left[\Delta P_b+V+\sum_n Vg_a^{n+1}V(\epsilon_a-E)^n\right.$$

$$\left.+\sum_{n,m}Vg_a^{n+1}Vg_a^{m+1}V(\epsilon_a-E)^{n+m}+\cdots\right]\psi. \tag{3.9}$$

The factors of $(\epsilon_a-E)$ on the right-hand side of this equation can be eliminated by iterating this equation. This is the final manipulation necessary to obtain a Raleigh-Schrödinger perturbation expansion.

Suppose that only even powers of $V$ occur on the right-hand side of Eq. (3.9). This special case occurs often in practice and we will deal with this case to fourth order to illustrate the technique. The general case will be recorded in the Appendix. So, in this case,

$$\mathcal{U}(E)=\Delta P_b+VG(E)V+VG(E)VG(E)VG(E)V+\cdots, \tag{3.10}$$

and Eq. (3.9) becomes

$$(E-\epsilon_a)\psi=\left[\Delta P_b+\sum_n Vg_a^{n+1}V(\epsilon_a-E)^n\right.$$

$$\left.+\sum_{n,m,l}Vg_a^{n+1}Vg_a^{m+1}Vg_a^{l+1}V(\epsilon_a-E)^{n+m+l}\right]\psi. \tag{3.11}$$

But this expression can be iterated by replacing $(\epsilon_a-E)$ by $\mathcal{U}(E)$, as given by Eq. (3.10), on the right-hand side,

$$(E-\epsilon_a)\psi=\left\{\Delta P_b+\sum_n Vg_a^{n+1}V\left[\Delta P_b+\sum_m Vg_a^{m+1}V(-\Delta P_b)^m\right]^n(-1)^n+\sum_{n,m,l}Vg_a^{n+1}Vg_a^{m+1}Vg_a^{l+1}V(-\Delta P_b)^{n+m+l}\right\}\psi, \tag{3.12}$$

where we have used Eq. (3.8) and have only collected terms to fourth order in $V$. The infinite sums in Eq. (3.12) will now be done explicitly. In the second term of Eq. (3.12) we meet the sum

$$\sum_{m=0}^{\infty}g_a^{m+1}(-1)^m\Delta^m=g_a\sum_{m=0}^{\infty}(-1)^mg_a^m\Delta^m$$

$$=\frac{g_a}{1+\Delta g_a}=\frac{Q}{g_a^{-1}+\Delta}$$

$$=\frac{Q}{\epsilon_a-H_0+\Delta}=\frac{Q}{\epsilon_b-H_0}=g_b. \tag{3.13}$$

So, to second order in $V$, Eq. (3.10) becomes

$$\mathcal{U}(E)=\Delta P_b+VG(E)V+\cdots$$

$$=\Delta P_b+\sum_m Vg_a^{m+1}V(-\Delta P_b)^m$$

$$=\Delta P_b+Vg_aV+\sum_{m\geq 1}Vg_a^{m+1}V(-1)^m\Delta^mP_b$$

$$=\Delta P_b+Vg_aVP_a+\sum_{m=0}Vg_a^{m+1}V(-1)^m\Delta^mP_b$$

$$=\Delta P_b+Vg_aVP_a+Vg_bVP_b, \tag{3.14}$$

where we have carefully dealt with the $m=0$ term in the sum and have inserted $1=P_a+P_b$ in the fourth line of this manipulation [since $\mathcal{U}(E)$ acts within the low-energy subspace this replacement is correct]. Now Eq. (3.12) reduces to

$$(E-\epsilon_a)\psi=\left\{\Delta P_b+\sum V(-1)^ng_a^{n+1}V(\Delta P_b+Vg_bVP_b+Vg_aVP_a)^n\right.$$

$$\left.+\sum V(-1)^ng_a^{n+1}V(-1)^mg_a^{m+1}\times V(-1)^lg_a^{l+1}V(\Delta P_b)^{n+m+l}\right\}\psi. \tag{3.15}$$

First, simplify the second term on the right-hand side of this equation. To second order in $V$,

$$(\Delta P_b+Vg_bVP_b+Vg_aVP_a)^n$$

$$=\Delta^nP_b+\delta_{n0}P_a+n\Delta^{n-1}P_bVg_bVP_b+\Delta^{n-1}P_aVg_aVP_b+\Delta^{n-1}P_bVg_aVP_a+\delta_{n1}P_aVg_aVP_a, \tag{3.16}$$

where we have used simple properties of projection operators to collect terms. The final sums

making up the second term are essentially just geometric series. After some algebra, this term becomes

$$Vg_bVP_b + Vg_aVP_a - Vg_b{}^2VP_bVg_bVP_b - Vg_a{}^2VP_aVg_aVP_a - Vg_ag_bVP_bVg_aVP_a - Vg_ag_bVP_aVg_bVP_b. \quad (3.17)$$

In the last term of Eq. (3.15) we meet the expression

$$P_b{}^{n+m+l} = \begin{cases} 1 \times \delta_{n+m+l,0} \\ P_b, \text{ otherwise}, \end{cases} \quad (3.18)$$

and the sums are the same as in Eq. (3.13), so we find

$$Vg_aVg_aVg_aVP_a + Vg_bVg_bVg_bVP_b. \quad (3.19)$$

Collecting all this we have our desired result,

$$\begin{aligned} E\psi = (&\epsilon_aP_a + \epsilon_bP_b + Vg_bVP_b + Vg_aVP_a \\ &+ Vg_aVg_aVg_aVP_a + Vg_bVg_bVg_bVP_b \\ &- Vg_b{}^2VP_bVg_bVP_b - Vg_ag_bVP_aVg_bVP_b \\ &- Vg_a{}^2VP_aVg_aVP_a - Vg_ag_bVP_bVg_aVP_a)\psi. \end{aligned} \quad (3.20)$$

Equation (3.20) gives the Raleigh-Schrödinger matrix perturbation theory for the eigenvalues $E_j$. Clearly the projection operators $P_a$ and $P_b$ serve to organize the $2 \times 2$ matrix structure of this equation. The reader will probably find it useful to write Eq. (3.20) directly as a $2 \times 2$ matrix. The generalization of Eq. (3.20) to cases in which odd powers of $V$ occur in $\mathfrak{V}(E)$ is handled in a similar way, and the resulting formula is recorded in the Appendix.

Some comments concerning this result and its derivation should be made. In the derivation we partitioned $H$ into two pieces $\hat{H}_0$ and $\hat{V}$ so that both $|\phi_a\rangle$ and $|\phi_b\rangle$ had eigenvalues $\epsilon_a$ when operated on by $\hat{H}_0$. One can check that this particular arrangement was not significant and that Eq. (3.20) follows in general. For example, we might have chosen $H = \hat{H}_0^1 + \hat{V}^1$ where $\hat{H}_0^1 = H_0 + \Delta P_a$ and $\hat{V}^1 = \lambda V - \Delta P_a$ and still have arrived at Eq. (3.20). Another nontrivial check of the scheme is made by assuming that $\epsilon_a = \epsilon_b$. Then Eq. (3.20) reduces to ordinary degenerate perturbation theory. [Degenerate perturbation theory follows trivially from Eq. (2.15) because then the zeroth-order $\epsilon$ matrix is proportional to the identity.]

It has probably occurred to the reader to ask if Eq. (3.20) could not have been obtained more directly. After all, it involves simple resolvents $g_a$ and $g_b$, so one would guess that the summations such as Eq. (3.13) could be avoided if the original problem were better formulated. This is, in fact, the case.[10] After using this formalism for some time on lattice gauge theory calculations, it was pointed out to us that this type of perturbation theory is used in nuclear and atomic physics for the same reasons we developed it here.[9] It has also been studied by mathematical physicists who have established useful results and properties we will quote below. In the realm of nuclear physics it is referred to as the "effective operator" method. The mathematical physics studies have supplied several useful results which we discuss briefly:

(1) Note that the $2 \times 2$ matrix in Eq. (3.20) is not Hermitian. This implies that the eigenvectors $\psi_1$ and $\psi_2$ will not in general be orthogonal. However, this result is not unexpected. Since $\psi_1$ ($\psi_2$) is the projection of the full state vector $|\psi\rangle$ ($|\psi_2\rangle$) into the low-energy subspace, the fact that $|\psi_1\rangle$ and $|\psi_2\rangle$ must be orthogonal if they have different energies, does not imply that $\psi_1$ and $\psi_2$ are orthogonal. However, since $E_1$ and $E_2$ are the energies of a problem which is explicitly Hermitian on the full Hilbert space, we are assured that the $E_i$ are real. It can be shown that the $2 \times 2$ problem can be replaced by an explicitly Hermitian one.[14] The perturbation theory then has additional terms and will not be discussed here. It may, however, be useful in the future.

(2) Particle masses are intensive quantities while the vacuum energy is extensive. These simple facts are not manifest even in the simplest Raleigh-Schrödinger perturbation expansions for field theories with nontrivial vacuum fluctuations. However, Raleigh-Schrödinger perturbation theory does have these properties and it is the various complicated terms in Eq. (3.20) which are essential here. A direct proof of these properties is best made by developing a connected perturbation formalism. Such a formalism exists for Eq. (3.20).[9,10] In field theory calculations one can also check that the $2 \times 2$ matrix of Eq. (3.20), when calculated relative to the vacuum energy, is intensive or, at least, has intensive eigenvalues.

## IV. THE CONTINUUM LIMIT AND MATRIX PADÉ APPROXIMANTS

The Hamiltonians for lattice field theories, certain spin systems, and even potential models have the property that the expansion parameter $\lambda$ diverges in the continuum limit. Extrapolation methods such as the Padé approximant have been used to continue the perturbation series beyond its radius of convergence and obtain estimates of the energy spectrum of the continuum problem of real interest.[1-6] The calculations have mainly dealt with mass ratios or dimensionless matrix elements—quantities which should have finite values in the continuum limit. Then diagonal Padé approximants could be formed from the strong-coupling

series and the continuum limit ($\lambda \to \infty$) could be taken directly. More sophisticated and reliable procedures have been suggested and applied to models to obtain more quickly convergent sequences of approximants. In the procedure described in Ref. 15, one forms the $[N/N]$ Padé approximant for a strong-coupling series of $2N$ terms and finds a value for the expansion parameter $\lambda_N$ where the approximant is to be evaluated. A successful recipe for choosing $\lambda_N$ equates it with the distance from the origin of the most distant pole in the $[N/N]$ approximant. This procedure can even generate sequences of approximants for functions with essential singularities at infinity.[15]

Clearly we need a generalization of the Padé approximant to matrices. Luckily "matrix Padé approximants" exist and have good mathematical properties.[11,12] We will review the definition of a matrix approximant and list some of its properties here. Given a series for a matrix function,

$$M(\lambda)=\sum M_j\lambda^j, \tag{4.1}$$

where $M_j$ are matrix coefficients, one can form a $[L/M]$ matrix Padé approximant,

$$M(\lambda)=P_L(\lambda)Q_M^{-1}(\lambda)+O(\lambda^{L+M+1}), \tag{4.2}$$

where $P_L$ and $Q_M$ are matrices. The coefficients in the matrices $P_L$ and $Q_M$ are obtained by the obvious generalization of the procedure used for ordinary approximants. Since $P_L$ and $Q_M$ do not commute, it is natural to ask whether the matrix approximant is unique. This is true and a proof which parallels the proof of the uniqueness of ordinary approximants can be found in Ref. 11.
Other useful properties of ordinary approximants generalize to matrix approximants. Recall the "duality" theorem[11] of ordinary approximants.

*Theorem*: If $P_L(\lambda)/Q_M(\lambda)$ is the $[L/M]$ Padé approximant to $f(\lambda)$, then $Q_M(\lambda)/P_L(\lambda)$ is the $[M/L]$ approximant to $1/f(\lambda)$ if $f(0)\neq 0$. The generalization reads

$$[L/M]_{T^{-1}}=[M/L]_T^{-1}, \tag{4.3}$$

where $T$ is the matrix to be approximated, and $T$ is assumed to be invertible. Another property which lies at the heart of the fast convergence of sequences of diagonal approximants is their invariance under Euler transformations.[11]

*Theorem*: If $P_M(\lambda)/Q_M(\lambda)$ is the $[M/M]$ Padé approximant to $f(\lambda)$, then $P_M(z)/Q_M(z)$ is the $[M/M]$ approximant to $f(z)$ where $z=A\lambda/(1+B\lambda)$. The generalization of this theorem to matrix Padé approximants holds identically.

Matrix Padé approximants have some special properties which we will list:

(1) Matrix approximants are basis independent.[12] In other words, if the matrix $M(\lambda)$ undergoes a similarity transformation, then its matrix approximants undergo the same similarity transformation. This is important, because it means that in our applications we can set up the low-energy subspace $S_L$ in any basis we please and always obtain the same energy eigenvalues.

(2) The matrix approximants to a Hermitian analytic matrix $[A^\dagger(\lambda^*)=A(\lambda)]$ are also Hermitian analytic.[11]

(3) Diagonal matrix approximants to a unitary matrix are unitary.[11]

In conclusion, we will form approximants for the masses of the particles in the low-energy subspace $S_L$ by computing its mass matrix in strong-coupling perturbation theory. A dimensionless matrix Taylor series will then be obtained by dividing through by an ordinary Taylor series for a "reference" particle. This must be done in order to obtain a matrix series which has a finite value in the continuum limit. Then the matrix series will be replaced by a sequence of matrix Padé approximants. The naive continuum limit $\lambda \to \infty$ can then be taken, or a more sophisticated sequence of approximants using the methods of Ref. 15 can be made.

## V. AN EXAMPLE OF THE METHOD-THE LINEAR POTENTIAL

We will illustrate this calculational method in a simple potential model. Field-theoretic calculations are in progress and will be reported elsewhere.[16] Potential models provide a nontrivial testing ground for this technique since the most naive strong-coupling methods produce rather erratic sequences of estimates for the energy levels.[17] We will present an example here where the matrix methods produce improved results allowing a naive continuum limit to be taken directly.

First, consider a lattice version of the Schrödinger equation for a linear potential,

$$H=-\frac{1}{2m}\frac{\partial^2}{\partial x^2}+\gamma|x|, \tag{5.1}$$

in one spatial dimension. There are many ways of placing this theory on a lattice. We choose the method shown in Fig. 1 where the lattice spacing is denoted $a$ and the minimum of the potential lies between two lattice sites. The discrete form of the second derivative is chosen to be the most naive form,

$$\frac{d^2}{dx^2}f(x)=\frac{1}{a^2}[f(x+a)+f(x-a)-2f(x)], \tag{5.2}$$

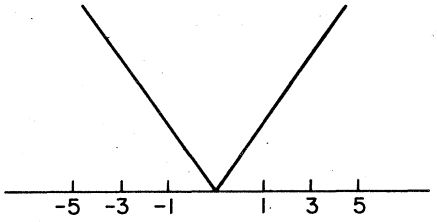


FIG. 1. The lattice version of the linear potential.

and the lattice is labeled by odd integers so the linear potential is replaced by

$$|x| = |n|a, \quad n = \pm 1, \pm 3, \pm 5, \ldots . \tag{5.3}$$

It is convenient to introduce "shift" operators

$$d^+ f(x) = f(x+a), \quad d^- f(x) = f(x-a). \tag{5.4}$$

The Hamiltonian now becomes

$$H = -\frac{1}{2ma^2}(d^+ + d^- - 2) + \gamma |n| a. \tag{5.5}$$

It is convenient to introduce a dimensionless operator,

$$W = \frac{1}{\gamma a} H = |n| - x(d^+ + d^-) + 2x, \tag{5.6}$$

where $x = (2m\gamma a^3)^{-1}$. We do perturbation theory in the kinetic energy,

$$W = W_0 + 2x - xV, \tag{5.7}$$

where

$$W_0 = |n|, \quad V = d^+ + d^-. \tag{5.8}$$

On a coarse lattice $x$ is very small and we can use it as an expansion parameter. Since $x$ diverges in the continuum limit, we must use extrapolation methods to deduce continuum results from these calculations.

Consider the spectrum of this lattice potential model. In the strong-coupling limit ($x = 0$), the $W$-energy operator is diagonalized by placing the particle on a particular site. Since sites $\pm|n|$ have the same value of $W_0$, the eigenstates naturally fall into two classes: those with symmetric wave functions and those with antisymmetric wave functions. Using the notation $|n\rangle$, the strong-coupling ground state is

$$\frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle). \tag{5.9a}$$

The first excited state is

$$\frac{1}{\sqrt{2}}(|1\rangle - |1\rangle). \tag{5.9b}$$

The perturbation $V$ does not mix states with different symmetries. We will obtain the energy of the first excited state of this model by computing the mass matrix in a truncated subspace of the space of all antisymmetric states. The subspace $S_L$ will consist of just the two lowest lying antisymmetric states, Eq. (5.9b) and

$$\frac{1}{\sqrt{2}}(|3\rangle - |-3\rangle). \tag{5.9c}$$

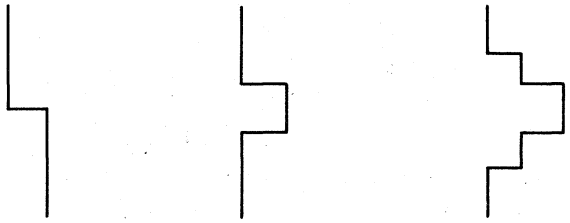


FIG. 2. Perturbation theory graphs: (a) first-order mixing, (b) second-order effect, and (c) fourth-order effect.

In the notation of Sec. III the state of Eq. (5.9b) will be denoted $|a\rangle$ and that of Eq. (5.9c) $|b\rangle$. The effective potential $\mathfrak{V}(E)$ will be computed in Raleigh-Schrödinger form to fourth order in $V$. Since odd orders of $V$ contribute to $\mathfrak{V}(E)$, the formula in the Appendix must be used.

We now sketch the calculations. The zeroth-order contribution is obviously

$$\epsilon_a P_a + \epsilon_b P_b = \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix}. \tag{5.10a}$$

It is convenient to visualize elements of the perturbation theory calculation with figures. In Fig. 2(a) we depict the single action of $d^-$—it moves the particle one unit to the left. It is easy to obtain the first-order mixing among the states,

$$PVP = x \begin{bmatrix} 1 & -1 \\ -1 & 0 \end{bmatrix}. \tag{5.10b}$$

In second order, graphs resembling Fig. 2(b) contribute. For example, if the particle is on site 3, $V$ can move it to site 5 or site 1. However, the resolvents $g_a$ and $g_b$ contain projection operators onto the high-energy subspace, so only the sequence of steps $3 \to 5 \to 3$ can contribute. The $g_b$ energy denominator for this transition is $(3-5)^{-1} = -\frac{1}{2}$. The total second-order contribution is

$$PVg_bVP_b + PVg_aVP_a = \begin{bmatrix} 0 & 0 \\ 0 & -1/2 \end{bmatrix}, \tag{5.10c}$$

where the second term on the left-hand side vanishes identically. Third- and fourth-order effects are calculated similarly. For example, a non-

vanishing third-order contribution is

$$-PVg_a{}^2VPVP=\begin{bmatrix}0&0\\0&1/16\end{bmatrix}\begin{bmatrix}1&-1\\-1&0\end{bmatrix}=\begin{bmatrix}0&0\\1/16&0\end{bmatrix}. \tag{5.10d}$$

In fourth order, graphs such as Fig. 2(c) contribute,

$$PVg_bVg_bVg_bVP_b=\begin{bmatrix}0&0\\0&-1/16\end{bmatrix}. \tag{5.10e}$$

Additional simple calculations provide all the terms in $\mathfrak{V}(E)$. Collecting all these calculations gives

$$E\psi=\left[\begin{bmatrix}1&0\\0&3\end{bmatrix}+x\begin{bmatrix}3&-1\\-1&2\end{bmatrix}+x^2\begin{bmatrix}0&0\\0&-1/2\end{bmatrix}+x^3\begin{bmatrix}0&0\\1/8&0\end{bmatrix}+x^4\begin{bmatrix}0&0\\1/32&0\end{bmatrix}\right]\psi. \tag{5.11}$$

We also need the strong-coupling expansion for the ground-state Eq. (5.9a),

$$E_0=1+x-\tfrac{1}{2}x^2+\tfrac{1}{4}x^3-\tfrac{1}{16}x^4+\cdots. \tag{5.12}$$

A nontrivial check on the algebra done in obtaining Eq. (5.11) can be made by finding the lowest eigenvalue of the matrix and expanding the resulting square root in powers of $x$. The resulting power series must be identical to the simple strong-coupling expansion of the energy $E_1$ of the first excited state, Eq. (5.9b). But the series for $E_1$ can be computed directly,

$$E_1=1+3x-\tfrac{1}{2}x^2-\tfrac{1}{4}x^3-\tfrac{1}{16}x^4, \tag{5.13}$$

and the agreement is easily verified. Of course, Eq. (5.11) has the advantage that the mixing between the two lowest antisymmetric states is treated exactly, while in Eq. (5.13) it is not.

Now we extract some results. First, truncate the series Eqs. (5.11) and (5.12) at second order. Dividing Eq. (5.11) by Eq. (5.12) gives

$$(E/E_0)\psi=\left[\begin{bmatrix}1&0\\0&3\end{bmatrix}+x\begin{bmatrix}2&-1\\-1&-1\end{bmatrix}+x^2\begin{bmatrix}-3/2&+1\\+1&2\end{bmatrix}\right]\psi. \tag{5.14}$$

We form the [1/1] matrix Padé approximant to the right-hand side. It is useful to record the general formula for this manipulation. Suppose we have a series

$$M=m_0+m_1x+m_2x^2, \tag{5.15}$$

where the coefficients are matrices. Then the [1/1] matrix Padé approximant to $M$ is

$$[1/1]_M(x)=m_0+xm_1(m_1-xm_2)^{-1}m_1, \tag{5.16}$$

as the reader can easily verify. Therefore,

$$\lim_{x\to\infty}[1/1]_M(x)=m_0-m_1m_2{}^{-1}m_1. \tag{5.17}$$

Applying this algebra to Eq. (5.14) gives

$$\lim_{x\to\infty}[1/1](x)=\tfrac{1}{8}\begin{bmatrix}29&-9\\-9&21\end{bmatrix}, \tag{5.18}$$

whose lowest eigenvalue is

$$E_1/E_0\approx\tfrac{1}{8}[25-(16+81)^{1/2}]\approx 1.894. \tag{5.19}$$

The exact answer for $E_1/E_0$ is 2.30, so the matrix method is 17% low. The ordinary Padé approximants give the estimate 3 for this ratio, so the matrix method has reduced the fractional error by almost a factor of 2.

Now consider Eqs. (5.11) and (5.12) to fourth order. The matrix equation for $E/E_0$ becomes

$$(E/E_0)\psi=\left[\begin{bmatrix}1&0\\0&3\end{bmatrix}+x\begin{bmatrix}2&-1\\-1&-1\end{bmatrix}+x^2\begin{bmatrix}-3/2&1\\1&2\end{bmatrix}+x^3\begin{bmatrix}9/4&-3/2\\-11/8&-13/4\end{bmatrix}+x^4\begin{bmatrix}-55/16&9/4\\69/32&75/16\end{bmatrix}\right]\psi. \tag{5.20}$$

We now replace the right-hand side of this equation by the [2/2] matrix Padé approximant. It is again useful to record the [2/2] matrix Padé for a general series,

$$M=m_0+m_1x+m_2x^2+m_3x^3+m_4x^4. \tag{5.21}$$

Then,

$$[2/2]_M=(1+\beta_1x+\beta_2x^2)^{-1}(\alpha_0+\alpha_1x+\alpha_2x^2), \tag{5.22}$$

where the matrices $\beta_i$ and $\alpha_i$ are obtained from the matrices $m_i$,

$$\begin{aligned}\alpha_0&=m_0,\\ \beta_1&=(m_4m_2{}^{-1}-m_3m_1{}^{-1})(m_2m_1{}^{-1}-m_3m_2{}^{-1})^{-1},\\ \beta_2&=(m_4m_3{}^{-1}-m_3m_2{}^{-1})(m_1m_2{}^{-1}-m_2m_3{}^{-1})^{-1},\\ \alpha_1&=m_1+\beta_1m_0,\\ \alpha_2&=m_2+\beta_1m_1+\beta_2m_0.\end{aligned} \tag{5.23}$$

So,

$$\lim_{x\to\infty}[2/2]_M(x)=\beta_2{}^{-1}\alpha_2. \tag{5.24}$$

Performing the matrix calculations for Eq. (5.20) gives

$$\lim_{x\to\infty}[2/2](x)=\begin{bmatrix}33.87690 & -11.37838\\ -7.31060 & 4.81087\end{bmatrix}. \quad (5.25)$$

The lowest eigenvalue of this matrix is

$$E_1/E_0\approx 19.34389-17.15784=2.18605\,, \quad (5.26)$$

which is just 5% below the exact answer. This result should also be compared against the ordinary [2/2] Padé approximant estimate for this mass ratio. It is 3.286 which is 62% above the correct answer. This example illustrates the fact that the ordinary Padé approximant gives a slowly convergent sequence of approximations in potential theory.[17] One method of speeding the convergence is that of Ref. 15 in which an optimal $x_N$ is chosen at every order $N$. This procedure works well, but the matrix method allows the naive $x\to\infty$ limit to be taken directly. One can also apply the $x_N$ method to the matrix calculations. It does not change the estimates substantially.

It is clear that the reason the matrix method works well is that it produces a better wave function for the first excited state than the most naive method. Since the first excited state has a node, the state must extend over several lattice sites before a lattice calculation of its energy will be reliable. By accounting for the mixing in the low-energy subspace nonperturbatively, we can achieve this.

## VI. CONCLUDING REMARKS

Application of these methods to field theory spectrum calculations have begun. An application to the Schwinger model will be discussed elsewhere.[16] The reason we are hopeful that the method will produce good results in (3+1)-dimensional lattice quantum chromodynamics is that particle states with realistic short-distance components can now be incorporated into a systematic strong-coupling procedure. We hope that our understanding of the pion, the $\eta$, and the $\Delta$-nucleon splitting will be improved by these efforts.

## ACKNOWLEDGMENTS

One of us (A. C.) wishes to thank his colleagues at the Centre d'Etudes Nucleaires, Saclay where this work was done. J. K. thanks Leonard Susskind for discussions and the encouragement to test matrix perturbation theory in potential models. He thanks J. Shigemitsu and P. N. Scharbach for checking the calculations. He thanks D. K. Sinclair, D. R. T. Jones, R. Kenway, and G. Frye for useful conversations and correspondence.

This work of J. B. K. was supported in part by the National Science Foundation under Grant No. NSF PHY 77-2579.

## APPENDIX

The generalization of Eq. (3.20) to the case where odd orders of $V$ contribute to the effective potential will now be recorded. The derivation using the methods of the text is straightforward but tedious. Using the same notation as the text [in which $\Delta=\epsilon_b-\epsilon_a$, $g_a=(1-P_a-P_b)/(\epsilon_a-H_0)$, $g_b=(1-P_a-P_b)/(\epsilon_b-H_0)$ we find

$$\begin{aligned}E\psi=[&\epsilon_aP_a+\epsilon_bP_b+PVP+PVg_bVP_b+PVg_aVP_a+PVg_bVg_bVP_b\\
&+PVg_aVg_aVP_a-PVg_a{}^2VPVP+\Delta PVg_a{}^2g_bVPVP_b+\Delta PVg_a{}^2g_bVP_bVP\\
&-\Delta^2PVg_a{}^2g_b{}^2VP_bVP_b+PVg_aVg_aVg_aVP_a+PVg_bVg_bVg_bVP_b-\Delta PVg_a{}^3g_bVP(PVPVP_b+P_bVPVP+PVP_bVP)\\
&+\Delta^2PVg_a{}^3g_b{}^2VP(P_bVPVP_b+P_bVP_bVP+PVP_bVP_b)\\
&-\Delta^3PVg_a{}^3g_b{}^3VP_bVP_bVP_b-PVg_b{}^2VP_bVg_bVP_b-PVg_a{}^2VP_aVg_aVP_a\\
&-PVg_ag_bVP_aVg_bVP_b-PVg_ag_bVP_bVg_aVP_a-PVg_a{}^2Vg_aVPVP\\
&-PVg_aVg_a{}^2VPVP+PVg_a{}^3VPVPVP+\Delta(PVg_bVg_a{}^2g_bVP+PVg_ag_bVg_a{}^2VP+PVg_a{}^2g_bVg_aVP)(PVP_b+P_bVP)\\
&-\Delta^2(PVg_a{}^2Vg_a{}^2g_bVP+PVg_bVg_a{}^2g_b{}^2VP+PVg_ag_b{}^2Vg_a{}^2VP+PVg_a{}^2g_b{}^2Vg_aVP)P_bVP_b]\psi\end{aligned}$$

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*Present address: Etec Corporation, 3392 Investment Blvd., Hayward, Calif. 94545.

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