

Convergent methods for calculating thermodynamic Green functions

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A convergent method of approximating thermodynamic Green functions is outlined briefly. The method constructs a sequence of approximants which converges independently of the strength of the Hamiltonian's coupling constants. Two new concepts associated with the approximants are introduced: the resolving power of the approximation, and conditional creation (annihilation) operators. These ideas are illustrated on an exactly soluble model and a numerical example. A convergent expression for the scattering rate in a field theory is also derived.

I. INTRODUCTION

The Feynman diagrammatic expansions¹ of Green functions have long exerted a dominant influence on theoretical physics. This strong influence continues even though it is well known that these series expansions in powers of the coupling constants usually do not converge.² The complete set of diagrams do of course account for every contribution to the Green function and the complete resummation of all of the diagrams recovers the exact Green function. The only problem is that the usual sequence of approximants in which successively more complicated diagrams are grouped by orders in powers of the couplings cannot be guaranteed to converge (for typical couplings) until the whole set has been assembled. In other words, even though the whole set of diagrams can be resummed formally to recover the exact Green function, no finite number of diagrams can be guaranteed to be any closer to the exact result than any other until the whole set of contributions has been evaluated and all of the cancellations realized.

This paper will present an outline of a synthesis of several well known mathematical relationships which yields a sequence of Green function approximants, converging for all values of the coupling strengths of the Hamiltonian. The method combines matrix techniques with algebraic methods to determine a sequence of convergent approximants to the Fourier transform of the retarded Green function. The rate of convergence of approximants is characterized by an energy scale of resolution over which they are accurate. In the following discussions this energy scale is called the resolving power of the approximation in analogy to the Rayleigh criterion of physical optics.³ The essence of the convergence theorem is that, given a particular resolving power, there exists an approximant which will be as "close" as desired to the exact Green function for that and all higher approximants. One implication of the results to be described below is that specifying a relatively large energy scale below which spectral detail is unimportant can lead to convergence of the sequence of approximants rather quickly.

One of the new features of this method will be the different manner in which the essential physical elements of an approximation are described. The usual method of

enumerating the types of Feynman diagrams which are included will not by itself prove to be appropriate since the approximants do not collect the interaction terms in the same fashion, and they certainly do not keep all contributions of the interactions to the same order in the couplings. It is necessary to introduce other means by which to characterize the elementary excitations included in an approximation. One tool for doing this is provided by conditional creation (annihilation) operators. As described below these operators represent events which occur only under particular constraints, as part of an elementary excitation. The number and type of these conditional operators included in an approximant will characterize it in much the same way that particular collections of diagrams have done so in perturbation theories.

The method to be described below is based primarily on the mathematical results of Masson⁴ and uses an important observation of Judd⁵ on Lie algebras. The synthesis presented here has some ties to the work of Feenberg,⁶ Hubbard,⁷ and one of the authors.⁸

The paper is divided into three main sections. Section II will exhibit the basic elements of the method including a description of the theorem by Masson which establishes the convergence of the approximants. The construction and use of conditional creation (annihilation) operators and other elements of the sequence of approximants will also be illustrated. In Sec. III the process of evaluating the sequence of approximants is discussed and a simple numerical example is studied which shows the different convergence properties of the standard diagrammatic approximants and the Feenberg-Masson approximants. Section IV will contain a rederivation of the usual scattering rate formulas from the perspective of this method. The results obtained bear some significant differences from the usual Born series and avoid many of the divergences in present-day methods. Finally in the Appendix the connection between conditional creation operators and Lie algebras is indicated.

II. GREEN FUNCTIONS AS RESOLVENTS IN AN OPERATOR SUPERSPACE

In the language of finite matrices, if \underline{H}_N is an $N \times N$ Hermitian matrix, then the matrix $z\underline{I}_N - \underline{H}_N$, where z is

a complex energy and I_N is the $N \times N$ matrix identity, is called the secular matrix of \underline{H} . The vanishing of the determinant of the secular matrix comprises the secular equation whose real roots determine the eigenvalues of \underline{H}_N . The resolvent $\underline{R}_N(z)$ of an operator or matrix \underline{H}_N is just the inverse operator or matrix inverse of the secular matrix:

$$\underline{R}_N(z) = (zI_N - \underline{H}_N)^{-1}. \quad (1)$$

Viewed as a complex function of z , the matrix elements of the resolvent are analytic functions of z away from the real axis and tend to zero like $1/z$ as the modulus of z tends to infinity away from the real axis. At points on the real axis where the eigenvalues of the matrix \underline{H} are found, the resolvent has poles. The matrix elements of the resolvent of an Hermitian operator with a continuous spectrum will exhibit a branch cut on the real axis in the region of the continuous spectrum.

It is generally well known that Green functions are closely related to matrix elements of the resolvent of Hamiltonian H :

$$R_{nn}(z) = \langle \Psi_n | (zI - H)^{-1} | \Psi_n \rangle. \quad (2)$$

The approximation of such resolvent matrix elements is the essential problem of many-body theory or field theory. In contrast to the usual methods of approximating the thermodynamic limit for such resolvent matrix elements, Masson's theorems⁴ give a method for approximating them with sequences of finite dimensional matrices which are guaranteed to converge. Because the focus of this paper is on applications of Masson's work, his proofs are not reproduced here but their main features are described. The essential result is that, for all complex z farther than a small distance δ from the real axis, and for any H whose domain is an infinite-dimensional Hilbert space, the resolvent matrix elements

$$R_{nn}(z) = \langle \Psi_n | (zI - H)^{-1} | \Psi_n \rangle \quad (3)$$

converge to the exact resolvent as the matrix size $N \rightarrow \infty$. More precisely, if ω is real and one can limit one's interest to some real δ in

$$R_{nn}(\omega + i\delta) = \langle \Psi_n | [(\omega + i\delta)I - H]^{-1} | \Psi_n \rangle, \quad (4)$$

then there is a matrix dimension $N(\delta)$ such that resolvents of matrices \underline{H}_N , where $N > N(\delta)$, give approximations to the exact corresponding resolvent matrix elements which are as good as you want for large enough N . In the Green-function context below it is convenient to think of δ as a measure of the resolution or resolving power of the approximation. One would expect that $N(\delta)$ would not have to be very large for large δ .

As we will attempt to illustrate below, the adoption of these matrix methods for the approximation of Green functions for many-body and field-theoretic model Hamiltonians should allow feasible approximations at useful levels of resolving power δ . The exciting part of Masson's theorems is that convergence is guaranteed independently of whether the coupling parameters are strong or weak. Ideas very closely related to the resolving power of the approximation have been developed for tridiagonal matrices

and continued fractions by Matsuda and Goda.⁹ They use the term "coarse graining."

The first step in our discussion is to focus on the retarded thermodynamic Green function for two second-quantized Fermi operators A and B , which can be written in the Zubarev¹⁰ notation as

$$\langle\langle A(t); B^\dagger(0) \rangle\rangle = -i \langle \{A(t), B^\dagger(0)\} \theta(t) \rangle, \quad (5)$$

where $\{\dots, \dots\}$ represents the anticommutator

$$\{A, B^\dagger\} = AB^\dagger + B^\dagger A \quad (6)$$

and $\langle(\dots)\rangle$ represents the thermal average with respect to the density matrix ρ in the grand canonical ensemble:

$$\langle(\dots)\rangle = \text{Tr}[\rho(\dots)]. \quad (7)$$

The function $\theta(t)$ is the unit step function.

It is straightforward to show⁸ that the time Fourier transform of (5) is equal to a special kind of matrix element of the resolvent of a Hermitian superoperator L which acts on a Hilbert space (superspace) of second-quantized Fermi operators:

$$\int_{-\infty}^{\infty} dt e^{i\omega t} \langle\langle A(t); B^\dagger(0) \rangle\rangle = ((B, (\omega + i\delta - L)^{-1} A)), \quad (8)$$

where the notation $((A, B))$ represents an inner product between second-quantized Fermi operators which are elements of a Hilbert space. This Fermi inner product is defined¹¹ as

$$((B, A)) = \langle \{A, B^\dagger\} \rangle = \langle AB^\dagger \rangle + \langle B^\dagger A \rangle \quad (9)$$

and will, in general, have a temperature and chemical-potential dependence derived from the density matrix in the grand canonical ensemble. In some cases these inner products will not be temperature dependent, but in most situations where there are many-particle intermediate states these inner products will depend on both temperature and chemical potential μ and must be evaluated self-consistently within each approximation or by using an approximate partition function.

The Hermitian superoperator L is essentially the quantum-mechanical Liouville operator and is defined to be that superoperator which takes any operator (superspace element) A into the commutator of A with the operator $K = H - \mu N$, where N is the total-particle-number operator:

$$LA = [A, K] = AK - KA. \quad (10)$$

In the usual treatments of Lie algebras these superoperators are called adjoint operators on the Lie algebra (usually with a minus sign).¹² The first description of these operators as "superoperators" seems to be due to Crawford and others.¹³ When the Hamiltonian H and the operators A and B are in second-quantized form, the determination of the inner products and the secular matrix of L in its $N \times N$ approximants reduces to a set of algebraic commutator and anticommutator evaluations.

The essence of our approximation method can now be stated in bare outline. To determine a particular matrix element of the resolvent of L , for example,

$((A, (z-L)^{-1}B))$, one chooses a resolving power δ and computes $N \times N$ secular matrices

$$((\phi_n, (zI - L)\phi_m))$$

with respect to an orthonormal basis set of N second-quantized operators ϕ_n , chosen to be a basis for expanding A and B (approximately) in the operator Hilbert space (superspace) and also chosen to make the secular matrix for L as diagonal as possible. For large enough N , the resolvents of these finite $N \times N$ truncations of the secular matrix for L with respect to a basis of many-particle operators are accurate approximations to corresponding matrix elements of the exact resolvent at $z = \omega + i\delta$. The physics and the art of a particular approximation reside in the selection of the orthonormal basis set ϕ_n of second-quantized operators. As we demonstrate below, these ϕ_n can be considered as conditional creation and annihilation operators, i.e., operators which create elementary excitations in certain states only if other simultaneous physical conditions are satisfied. We suggest that the interpretation and choice of these conditional creation (annihilation) operators in the basis set ϕ_n can determine approximations with much the same degree of physical understanding that diagrams have allowed. By decomposing the elementary excitations into certain linear combinations of conditional operators (determined in part by symmetries of the Hamiltonian), the nature of the important physical processes can be determined. In particular, the selection of the most important set of conditional creation operators will determine the essential physics in much the same way that diagram selection does now.

While the outline given above gives the essential features of this method, several features which are particularly important for approximate treatments of many-body problems need to be discussed further. Primary among these is that in the calculation of some secular matrices there will be matrix elements $((A, LB))$ which are themselves temperature dependent. Most of these will involve thermal averages of the form $\langle A^\dagger B \rangle$. This type of thermal average can always be evaluated if the spectral function can be determined. To simplify later expressions we write the spectral function as

$$F_\delta[(B, (\omega - L)^{-1}A)] = +i[(B, (\omega + i\delta - L)^{-1}A) - (B, (\omega - i\delta - L)^{-1}A)], \quad (11)$$

where ω is real and we have explicitly exhibited the δ (resolving power) dependence of the spectral function.

Using the standard properties¹⁴ of thermodynamic Green functions we have

$$\langle A^\dagger B \rangle = \lim_{\delta \rightarrow 0} \int d\omega f(\omega) F_\delta[(B, (\omega - L)^{-1}A)] / 2\pi, \quad (12)$$

where $f(\omega)$ is the usual Fermi function. While the exact formula (12) involves the limit as $\delta \rightarrow 0$, our strategy where necessary will be to evaluate $\langle A^\dagger B \rangle$ using a nonzero value of δ and an $N \times N$ truncation large enough to give us essentially exact results for that value of the resolving power.

Illustration of some parts of the method and the role of conditional creation operators can be made by looking at a simple model Hamiltonian which we can solve exactly. This Hamiltonian is the atomic-limit Hubbard Hamiltonian¹⁵

$$K = \epsilon_+ n_+ + \epsilon_- n_- + U n_+ n_- . \quad (13)$$

Here ϵ_+ and ϵ_- are one-electron energies with different spins (measured relative to the chemical potential), U is the Coulomb repulsion energy for the two-electron state, and n_s is the number operator for the single-particle state of spin s created by c_s^\dagger .

This model is a good example not only because it can be easily solved exactly, but also because, as apparently Hubbard is the first person to discover, it offers one of the simplest examples of conditional creation operators. Hubbard noted that

$$c_+ = (1 - n_-)c_+ + n_- c_+ \quad (14a)$$

and that the two operators in this sum diagonalize L :

$$L(1 - n_-)c_+ = \epsilon_+(1 - n_-)c_+, \quad (14b)$$

$$L n_- c_+ = (\epsilon_+ + U)n_- c_+. \quad (14c)$$

These two conditional annihilation operators are elements of the superspace of Fermi operators and are orthogonal but not normalized to unity. The relevant inner products are

$$(((1 - n_-)c_s, (1 - n_-)c_s)) = 1 - \langle n_- \rangle, \quad (15a)$$

$$((n_- c_s, n_- c_s)) = \langle n_- \rangle, \quad (15b)$$

$$(((1 - n_-)c_s, n_- c_s)) = 0. \quad (15c)$$

A straightforward application of these inner products and the definition of the resolvent yields the well known result that

$$((c_s, (\omega - L)^{-1}c_s)) = (1 - \langle n_- \rangle) / (\omega - \epsilon_s) + \langle n_- \rangle / (\omega - \epsilon_s - U). \quad (16)$$

These operators which diagonalize L are very simple conditional annihilation operators. The operator $n_- c_+$ will annihilate the spin-up electron only if there is also present a spin-down electron on the atom. Similarly, the operator $(1 - n_-)c_+$ will annihilate the spin-up electron only if there is not another spin-down electron on the atom.

The essential property which enabled us to diagonalize L in this case was the selectivity of the conditional annihilation operators: the two different events depending on the population of the opposite spin orbital were separated out. To study the properties of many-particle states in general one needs to select conditional annihilation operators that separate distinctly different physical events. The operators that are included in a particular approximation will represent a set of fundamentally correlated but distinct physical events which are coupled together by the Hamiltonian and the thermodynamic equilibrium.

For this simple model it may seem that the solution has been obtained by a simple trick and it is unclear that there

is anything systematic with which to make generalizations to more complicated systems. The optimal means of generalizing to more complicated systems was written down first by Judd¹⁶ in a different context. From his observations we can say that the conditional creation and annihilation operators will be the stepping operators of some large Lie algebra of type $U(M)$ for some M and that, if the algebra is represented by its maximal Cartan form,¹⁷ one achieves the representation with the most selectivity. This high level of selectivity enhances the ability to diagonalize the L operator. As described in the Appendix, the Hubbard atomic-limit conditional creation (annihilation) operators are part of a unitary algebra $U(4)$. It is also possible to write down the stepping operators for a general atomic shell following Judd. This method appears quite cumbersome at first, but it does make the diagonalization or near diagonalization of complicated Hamiltonians more tractable.

The Judd procedure constructs the Cartan form of the Lie algebra quite directly. First one defines a creation operator A_θ^\dagger which creates the full shell and defines a projection operator I_θ , the projection operator for the empty shell or shell vacuum,

$$I_\theta = A_\theta A_\theta^\dagger. \quad (17)$$

Next, one constructs creation operators $A_{\psi(n)}^\dagger$ for all of the n -electron states in the shell for all possible n values. The set of operators

$$\Phi_{nn'} = A_{\psi(n)}^\dagger I_\theta A_{\psi(n')}, \quad (18)$$

where $|\psi(n)\rangle$ and $|\psi'(n')\rangle$ are shell states of n and n' electrons, respectively, make up the Lie algebra associated with the shell and its states. The particular set of operators which annihilate one extra electron,

$$\Phi_n = A_{\psi(n)}^\dagger I_\theta A_{\psi(n+1)}, \quad (19)$$

are the class of one-electron conditional annihilation operators which can be used to construct the one-electron Green function for more complicated systems. Using the fundamental anticommutation relations between the one-particle operators in the shell, the Judd form of the stepping operators can be collapsed into a form like the Hubbard conditional operators, which form can often make the nature of the conditional events more transparent. [See (A7) in Appendix.] Actually, however, the Judd form of the stepping operators does describe the initial and final many-particle states directly and can be a very useful tool for the description of final-state effects in x-ray photoemission spectroscopy and other types of experiments. In more complicated problems the fact that these stepping operators are part of a large Lie algebra has not yet proven to be an essential property for constructing good approximations, but knowledge of the commutation and anticommutation relations for the canonical Cartan form of

the Lie algebra has made some symmetry considerations and some calculations easier. Some more information on the Lie algebra structure of the Hubbard atomic limit is also included in the Appendix.

An example of the use of these ideas for the solution of a more complicated but still soluble model is the treatment of another work¹⁸ which studies the Hubbard dimer model with Hamiltonian

$$H = \sum_s \epsilon_s (n_{1s} + n_{2s}) + U(n_{1+}n_{1-} + n_{2+}n_{2-}) + \sum_s t(c_{1s}^\dagger c_{2s} + c_{2s}^\dagger c_{1s}), \quad (20)$$

where the numbers 1 and 2 label two sites and s runs over the spin values $\pm\frac{1}{2}$. The Lie algebra for this Hamiltonian is $U(16)$, but only a small subset of the operators in the algebra was necessary for obtaining the thermodynamic properties of the system. The study of other model Hamiltonians using these ideas is underway, especially in the theory of valence fluctuations, and will be reported elsewhere.

III. SEQUENCES OF APPROXIMANTS

In this section the problem of constructing $N \times N$ approximants to resolvents is discussed. The strategy for constructing approximants as suggested by Masson's theorem requires some method of evaluating the matrix elements of the resolvent of the L operator. In many ways the examination of the existing analytic formulas for this process can be considered as a reconsideration of the earlier work of Feenberg¹⁹ on a "perturbation" theory which does not contain repeated factors of the off-diagonal matrix elements of the Hamiltonian. In order to review these analytic formulas and to examine several fine points of the construction of a convergent sequence of approximants for a specific level of resolving power δ , let us define the following matrix elements of L :

$$L_{nn'} = \delta_{nn'} E_n + V_{nn'}, \quad (21)$$

where $\delta_{nn'}$ is the Kronecker delta and we have used n and n' to represent the labels of some orthonormal basis set of the operator superspace.

The diagonal matrix elements of the resolvent of L are

$$\langle n | [(\omega + i\delta)I - L]^{-1} | n \rangle = [\omega + i\delta - e_n(\omega + i\delta)]^{-1}, \quad (22)$$

where

$$e_n(\omega) = E_n + \Sigma_n(\omega) \quad (23)$$

and $\Sigma_n(\omega)$ is the self-energy of the n th state which must be defined using the summation restrictions found in the usual expansion of determinants and in Feenberg's early work:

$$\Sigma_n(\omega) = \sum_{l(\neq n)} \frac{|V_{nl}|^2}{\omega - e_l(n; \omega)} + \sum_{\substack{l(\neq n) \\ l'(\neq n, l)}} \frac{V_{nl} V_{ll'} V_{l'n}}{[\omega - e_l(n; \omega)][\omega - e_{l'}(n, l; \omega)]} + \dots, \quad (24)$$

where the $e_l(n; \omega)$ and the $e_{l'}(n, l; \omega)$ are defined in the same way as $e_n(\omega)$, except that any state indices listed in front of

the semicolon cannot be included in the sums which define these "reduced" self-energies. For any $N \times N$ truncation of L the expression for the self-energy $\Sigma_n(\omega)$ will only contain a finite number of terms and the last term in the sum will contain N factors of V . This expression is, of course, simply another way of writing the formula for the nn element of an inverse matrix using the Laplace expansion in terms of signed minors.

In the same way the off-diagonal matrix elements of the resolvent can be written as

$$\langle n | (\omega - L)^{-1} | n' \rangle = [\omega - e_n(\omega)]^{-1} T_{nn'} [\omega - e_{n'}(n; \omega)]^{-1}, \quad (25)$$

where one can define a sum-restricted T matrix as

$$T_{nn'} = V_{nn'} + \sum_{l (\neq n, n')} \frac{V_{nl} V_{ln'}}{\omega - e_l(n, n'; \omega)} + \sum_{\substack{l (\neq n, n'), \\ l' (\neq n, n', l)}} \frac{V_{nl} V_{ll'} V_{l'n'}}{[\omega - e_l(n, n'; \omega)][\omega - e_{l'}(n, n', l; \omega)]} + \dots \quad (26)$$

This restricted T matrix is very close to the form of the T matrix that is usually defined for the Born series, but the summation restrictions play a very important role in restricting the poles and singularities of the T matrix. The summation restrictions also are important because they essentially assure the convergence of the approximants.

Using these analytic expressions we can write the substance of the Masson theorem as

$$\langle n | [(\omega + i\delta) - L]^{-1} | n' \rangle = \lim_{N \rightarrow \infty} [(\omega + i\delta) \underline{I}_N - \underline{L}_N]_{nn'}^{-1}. \quad (27)$$

The Masson theorem states essentially that it is the sequence of the matrix elements of the inverse matrices which converge to the exact matrix elements for a fixed distance off the real axis. To omit any of the terms in the analytic expressions (22) and (25) is to forfeit the guarantee of convergence unless such terms can be shown to be negligible.

As alternatives to summing the analytic expressions, several numerical methods suggest themselves as being useful. For relatively small matrices ($N < 100$) standard inversion routines would seem to be adequate, though increasingly time consuming as the matrices get larger. An alternative for very large matrices may be some version of the matrix inversion routines of Kuti²⁰ using Monte Carlo techniques. Recent preliminary work with these indicate that there are difficulties with convergence and reliability near isolated poles,²¹ but more work is necessary to confirm this on larger matrices.

As an example to illustrate the profound difference between the two types of approximations, i.e., the standard diagrammatic methods and the Feenberg-Masson sequence of approximants, let us now consider a case where a simple matrix represents an infinite Hamiltonian matrix. We will carry out the calculation of the self-energy of one of the lowest-lying states of this system at an energy for which the usual lowest-order contribution to the self-energy diverges logarithmically. Consider the infinite matrix with all of the off-diagonal elements equal to one. On the diagonal let the value of the n th element be equal to n . The energy of the lowest "unperturbed" energy is 1 and we will seek the value of the self-energy for this energy level at the frequency value $\omega = 0$. There is nothing special about this value except that it should not correspond to an exact energy of the system and so the convergence of the approximants at this point need not be limit-

ed to some finite distance off the real axis. The lowest-order Feynman-type expression for the self-energy at frequency ω for the lowest state is given by

$$\Sigma_1(\omega) = \sum_{n=2}^{\infty} 1/(\omega - n). \quad (28)$$

The worst place for this to be evaluated is at $\omega = 0$, although a similar behavior is expected at other values of ω . In order to apply the Masson theorem we need to take the inverses of $N \times N$ truncations of the Hamiltonian matrix and determine the self-energy at $\omega = 0$ using the formula

$$\Sigma_1^N(0) = 1 / \{ [(\underline{H}_N)^{-1}]_{11} - 1 \}. \quad (29)$$

In order to compare the two approximations on equivalent ground we can evaluate the first N terms of the Feynman sums for each truncation. If one compares the analytic expressions for the self-energy (24), one sees that only terms of the exact analytic expressions which involve the diagonal and the first row and column of the matrix are included in the lowest-order approximation.

The numerical comparison of the two sequences is shown in Fig. 1, where we have plotted the values of the two sequences versus the size of the truncated matrix. It is quite clear from the rapid growth in the lowest-order diagrammatic approximation that it does not contain the cancellations which are necessary in order to recover con-

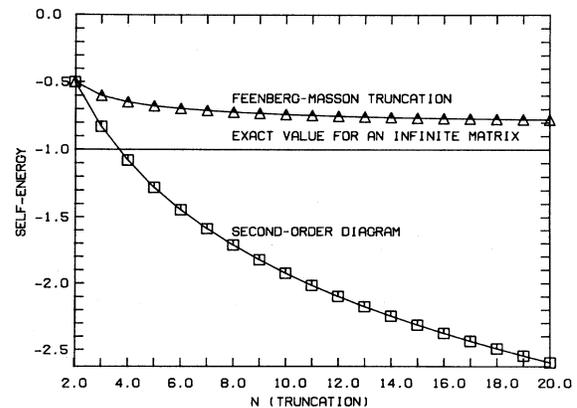


FIG. 1. Comparison of truncated approximants for a model self-energy in the Feenberg-Masson truncation and the simplest perturbation-theory approximation. The horizontal line at -1.0 is the exact value for this model.

vergence. The sequence represented by the Feenberg-Masson sequence is seen to converge steadily, but the convergence appears to be rather slow. Because this matrix can be inverted exactly for the sequence of truncations, it is possible to say that the convergence of the truncations is of order $1/\ln(N)$ and thus quite slow.

While this example does illustrate the inadequacy of the usual lowest-order diagrammatic approximations, it is somewhat disappointing that the truncation sequence does not converge faster. The example suggests the sequence of approximants outlined in this paper may be too slow for practical use, but it is necessary to remember that this example is very off-diagonal and the best approach to any problem will be to choose the set of states which will give as much diagonalization as possible during the treatment. The implications for field theory and many-particle systems which have been treated by the standard methods and found to exhibit divergent approximations should also be clear. Masson's theorem in this application suggests that most if not all of the usual divergences are symptomatic of the approximation method. In particular, methods which seek to renormalize the asymptotic series expansion may not be able to guarantee convergence of the renormalized theory to the exact result. On the other hand, application of the method outlined here to some of those models should yield convergent approximations free from these divergences. As a step toward that effort the next section will present a derivation of the scattering rate from the perspective of this convergent method.

IV. DERIVATION OF THE SCATTERING RATE

In this section a rederivation of the usual scattering formulas is given in a form that allows the immediate application of the truncation approximation methods outlined above. This means that the results carry the same guarantee of convergence which the Masson theorem gives to direct calculations of Green functions. The derivation also uses a slightly different set of mathematical theorems than usual and thus is able to avoid the use of products of delta functions and other elements of the standard derivation.²² The biggest difference between this derivation and the usual Born series is the presence here of the summation restrictions on the form of the T matrix.

The derivation is also couched in the language of single-particle fermion operators to allow use of earlier formulas of this paper. However, the generalization to more complex operators and bosons is immediate and straightforward.

The derivation begins with an expression for the initial state $|s\rangle$ and the final state $|r\rangle$ in terms of the vacuum state $|0\rangle$ and the appropriate creation operators:

$$\begin{aligned} |r(t)\rangle &= c_r^\dagger(t) |0\rangle, \\ |s(t')\rangle &= c_s^\dagger(t') |0\rangle, \end{aligned} \quad (30)$$

where the Heisenberg time dependence of the operators is implied.

The transition amplitude between state $|r\rangle$ at time t and state $|s\rangle$ at time zero is given by

$$\langle r(t) | s(0) \rangle = \langle c_r(t) c_s^\dagger(0) \rangle, \quad (31)$$

where we have indicated the ground-state average by $\langle \dots \rangle$. At this point it is worthwhile generalizing our starting point to particles created in a thermal bath rather than just from a ground state. To that end we consider transition amplitudes for averages defined by a density matrix for a grand canonical ensemble. At the limit of zero temperature and very large and negative chemical potential we can recover the ground-state scattering picture above.

Given a transition amplitude

$$\langle c_r(t) c_s^\dagger(0) \rangle = \text{Tr}[\rho c_r(t) c_s^\dagger(0)], \quad (32)$$

we seek to evaluate the transition rate w_{rs} which is the time derivative of the transition probability P_{rs} as t approaches $+\infty$, where

$$P_{rs} = |\langle c_r(t) c_s^\dagger(0) \rangle|^2. \quad (33)$$

Before calculating the time derivative let us note that there is a trivial time dependence of the transition amplitude (31) which is conveniently eliminated. This is the time behavior of $c_r(t)$ itself. In the case where there is no scattering potential, that time dependence is just an exponential factor $\exp(-i\epsilon_r' t)$, where ϵ_r' is the "free-particle" energy of the state $|r\rangle$. To eliminate this time behavior we consider the evaluation of probability amplitudes including a factor of $\exp(+i\epsilon_r' t)$:

$$\langle c_r(t) c_s^\dagger(0) \rangle_e = \exp(i\epsilon_r' t) \langle c_r(t) c_s^\dagger(0) \rangle. \quad (34)$$

We choose the value of ϵ_r' in the following to be the renormalized energy of the state created by c_r^\dagger . As can be seen, this will not change the transition probability and will get rid of a trivial time dependence. This factor accomplishes much of what the usual interaction representation was constructed to do.

The transition rate is evaluated from

$$w_{rs} = \langle c_r(t) c_s^\dagger(0) \rangle_e^* (d/dt) \langle c_r(t) c_s^\dagger(0) \rangle_e + \text{c.c.} \quad (35)$$

To compare with experiments we examine the values of w_{rs} as $t \rightarrow \infty$ and seek those contributions which do not tend to zero in that limit.

As discussed before, the calculation of these amplitudes can be easily accomplished if the spectral function of the corresponding thermodynamic Green function

$$g_{rs}(\omega) = ((c_s, (\omega - L)^{-1} c_r)) \quad (36)$$

is known. The spectral function

$$A_{rs}(\omega) = F[g_{rs}(\omega)] \quad (37)$$

can be used directly to calculate

$$\begin{aligned} \langle c_r(t) c_s^\dagger(0) \rangle_e &= \int d\omega A_{rs}(\omega) [1 - f(\omega)] \\ &\quad \times \exp[-i(\omega - \epsilon_r') t] / 2\pi. \end{aligned} \quad (38)$$

The Fermi function $f(\omega)$ appears because we are using the thermodynamic Green functions. For most real scattering situations the chemical potential of the beam particles is so low (negative) that the Fermi function is negligible for all ω of interest. The presence of this factor will not be of any direct significance in what follows.

The amplitudes we seek can all be expressed in the form

of the difference between two integrals $I(p, q)$, where p and q both take on values of $+1$ or -1 , of the form

$$I(p, q) = \int d\omega G_{pq}(\omega) \exp[-i(\omega - \epsilon'_r)t]/2\pi, \quad (39)$$

where the index p defines the factors for the transition amplitude and its derivative. The definition of G_{pq} is given by

$$G_{p\pm} = g_{rs}(\omega \pm i\delta)[1 - f(\omega)], \quad p = +1 \quad (40)$$

$$G_{p\pm} = -i(\omega - \epsilon'_r)g_{rs}(\omega \pm i\delta)[1 - f(\omega)], \quad p = -1 \quad (41)$$

and we have the following results for large time t :

$$\langle c_r(t)c_s^\dagger(0) \rangle_e = I(+, -) - I(+, +), \quad (42)$$

$$d/dt \langle c_r(t)c_s^\dagger(0) \rangle_e = I(-, -) - I(-, +). \quad (43)$$

Thus we seek to evaluate $I(p, q)$ for very large t as $\delta \rightarrow 0$. Any contributions which are independent of time in that regime will comprise our scattering amplitude.

The largest long-time contribution will come from poles which are close to the real axis. To evaluate their contributions assume that we can write $G_{p\pm}$ near one of these poles as

$$G_{p\pm}(\omega) = C_{p\pm}(\epsilon'_r)/(\omega \pm i\delta - \epsilon'_r). \quad (44)$$

In this case,

$$I(p, \pm) = C_{p\pm}(\epsilon'_r) \int d\omega e^{-i\omega t}/2\pi(\omega \pm i\delta). \quad (45)$$

For the scattering problem we are interested in $t > 0$, so the appropriate contour must lie in the lower half plane and we pick up residue only from the $+i\delta$ term. This means that the $I(p, +)$ integral will be nonzero and the $I(p, -)$ will be zero. We find that

$$I(p, +) = \lim_{t \rightarrow \infty} [C_{p+}(\epsilon'_r)e^{-\delta t}], \quad (46)$$

which is time independent in the limit of $\delta \rightarrow 0$ for large times t . The remaining steps in the derivation involve the determination of the residues C_{-+} and C_{++} . The distinction between this method and the standard method becomes most obvious at this point. The forms of the off-diagonal spectral function are taken from the analytic Feenberg forms (25) as required by the Masson theorem. The forms of the residues $C_{-+}(\epsilon'_r)$ can be obtained by remembering that the behavior of the prefactor and post-factor in (25) can be written as

$$[\omega - \epsilon_r - \Sigma_r(\omega)]^{-1} = (\omega - \epsilon'_r)^{-1} Z_r(\epsilon'_r), \quad (47)$$

where Z is the usual renormalization coefficient

$$Z_r(\epsilon'_r) = [1 - \partial/\partial\omega \Sigma_r(\epsilon'_r)]^{-1}.$$

The expression for the T matrix will be written as

$$T_{rs}(\epsilon'_r) = Z_r(\epsilon'_r) T_{rs}^0(\epsilon'_r) Z_s(\epsilon'_r), \quad (48)$$

where T_{rs}^0 is the restricted T matrix defined in (25). The residues are

$$C_{++}(\epsilon'_r) = T_{rs}(\epsilon'_r + i\delta)(\epsilon'_r + i\delta - \epsilon'_s)^{-1}, \quad (49)$$

$$C_{-+}(\epsilon'_r) = iT_{rs}(\epsilon'_r + i\delta), \quad (50)$$

so that the constant scattering rate as $t \rightarrow \infty$ is

$$w_{rs} = C_{++}^* C_{-+} + C_{++} C_{-+}^*,$$

where each C function is evaluated at $\epsilon'_r + i\delta$. Writing the residues as real and imaginary parts of each factor yields the standard expression

$$w_{rs} = 2 |T_{rs}(\epsilon'_r)|^2 \delta / [(\epsilon'_r - \epsilon'_s)^2 + \delta^2]. \quad (51)$$

While Eq. (51) has the same structure as the usual form of the scattering rate, there are several differences which should be noted. First, the energies and the T matrix are already renormalized in the sense of (46). Second, the T matrix definition explicitly contains summation restrictions over the intermediate sums of states. These summation restrictions are essential for the guarantee of convergence of the approximants. Third, this expression should yield convergent expressions for the scattering rate independently of the coupling strengths. Because these convergent approximants begin with exactly the same form as the lowest-order diagrammatic expansions, one should expect to recover the same selection rules and cross sections that the lowest-order contributions give in the diagrammatic methods.

V. SUMMARY

This paper has briefly outlined a convergent method for approximating thermodynamic Green functions. The approximations are formed by calculating the resolvents of truncated secular matrices in an operator space whose vectors are conditional creation (annihilation) operators. The theorem guaranteeing convergence implies that, for a fixed resolving power δ off the real energy axis, finite $N \times N$ matrix resolvents with N chosen large enough will yield an approximation as close to the exact Green function as desired for that value of $\omega + i\delta$. The approximations in this method are not easily characterized by noting the diagrams to which they correspond because each approximant will contain all of the diagrammatic contributions to the self-energy that must be present in an $N \times N$ matrix inverse. Furthermore, these approximants do not include all diagrams to a given order, but they include only those sum-restricted contributions which are demanded by the truncated inverse. As a relatively simple means of classifying the approximation it is useful to describe the subspace of conditional creation (annihilation) operators which are used as a basis for the truncated resolvent matrix employed to evaluate the one-particle Green function.

The rate of convergence of the sequence of approximants has not yet been studied for complicated many-particle models. In general, the convergence should be much faster for large values of the resolving power δ since large values leave little detail of the spectrum to be determined. These questions are being explored in several applications and will be reported elsewhere.

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APPENDIX: LIE ALGEBRAS AND CONDITIONAL CREATION (ANNIHILATION) OPERATORS

The conditional creation and annihilation operators discussed above belong to an algebra of operators, usually a Lie algebra of unitary type $U(n)$ for some large n . Some of the general properties of these Lie algebras can be important for the efficient construction of conditional operators in calculations. While all of the structure has not yet been shown to be useful for general many-particle systems, it is included for completeness.

There are two types of operators in a Lie algebra $U(n)$, orthogonal projection operators H_i and stepping operators ϕ . The projection operators commute among themselves and the largest set of these is called the maximal Cartan subalgebra. The number of these projection operators which are linearly independent is $n-1$. The sum of all n of the projection operators is the identity operator for the space on which the algebra operates:

$$I = \sum_{i=1}^n H_i . \quad (\text{A1})$$

The remaining elements of the Lie algebra are the stepping operators ϕ which we have also called conditional operators. In the standard treatments of Lie algebras the labels for the stepping operators are formed from the root vectors, n tuples α containing the eigenvalues α_i of ϕ in commutation with the i th projection operator H_i :

$$[H_i, \phi_\alpha] = \alpha_i \phi_\alpha, \quad \alpha = (\alpha_1, \alpha_2, \dots, \alpha_n) . \quad (\text{A2})$$

The standard notation for Lie algebras labels the stepping operators by their root vectors. While this is useful in some situations, different notation has been chosen here. Two other commutator equations comprise the remainder of the structure of the Lie algebra, for our purposes. These equations are

$$[\phi_\alpha, \phi_\alpha^\dagger] = \sum_{i=1}^n \alpha_i H_i , \quad (\text{A3})$$

$$[\phi_\alpha, \phi_\beta] = N_{\alpha\beta}^\gamma \phi_\gamma , \quad (\text{A4})$$

where the structure factor $N_{\alpha\beta}^\gamma$ is nonzero only if the sum of the root vectors α and β is also a root vector. These relationships are useful for determining the multiplication

table of the algebra.

The explicit representation of $U(4)$ appropriate to the Hubbard atomic-limit Hamiltonian (13) can be constructed using the Judd procedure. The many-electron states are $A^\dagger |0\rangle = c_+^\dagger c_-^\dagger |0\rangle, c_+^\dagger |0\rangle, c_-^\dagger |0\rangle$, and the vacuum state $|0\rangle$. The projection operator for the vacuum state of the shell is

$$I_\theta = c_- c_+ c_+^\dagger c_-^\dagger = (1 - n_-)(1 - n_+) = AA^\dagger . \quad (\text{A5})$$

The four commuting projection operators are

$$\begin{aligned} H_0 &= I_\theta , \\ H_1 &= c_+^\dagger I_\theta c_+ , \\ H_2 &= c_-^\dagger I_\theta c_- , \\ H_3 &= A^\dagger I_\theta A . \end{aligned} \quad (\text{A6})$$

The annihilation-operator form of the stepping operators of the algebra can be written out for different spin values along with their root vectors as follows:

$$\begin{aligned} I_\theta c_s &= (1 - n_{-s})c_s, \quad \alpha = (1, -1, 0, 0) \text{ and } s = +\frac{1}{2} \text{ or} \\ &\quad \alpha = (1, 0, -1, 0) \text{ and } s = -\frac{1}{2} , \\ c_{-s}^\dagger I_\theta A &= n_{-s}c_s, \quad \alpha = (0, 0, -1, 1) \text{ and } s = +\frac{1}{2} \text{ or} \\ &\quad \alpha = (0, -1, 0, 1) \text{ and } s = -\frac{1}{2} , \\ c_-^\dagger I_\theta c_+ , \quad &\alpha = (0, 1, -1, 0) , \\ I_\theta A , \quad &\alpha = (1, 0, 0, -1) . \end{aligned} \quad (\text{A7})$$

The first two stepping operators change the particle number by one and thus will span the space for the one-electron Green function, as implied in (14a). The last two correspond to zero- and two-particle change and will appear as factors of one-particle operators in more complicated conditional creation operators when hopping to other sites or hybridization terms are included in the Hamiltonian. Finally, from the structure of the Lie algebra it can be seen that any eigenvalue of L will be the difference between the eigenvalues of the Hamiltonian for the two states connected by the corresponding stepping-operator eigenvector of L .

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