A recursive solution of Heisenberg's equation and its interpretation

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Abstract. We present the generalization of the recursion method of Haydock and co-workers to systems of many interacting particles. This new method has close similarities to the memory function or Mori formalism, but with some important differences. Heisenberg's equation for the time evolution of a microscopic operator is recursively transformed into a tridiagonal matrix equation. This equation resolves the operator into components corresponding to transitions of different energies. The projected spectrum of transitions has a continued fraction expansion given by the elements of the tridiagonal matrix. We show that for an appropriate choice of inner product this density of transitions obeys a generalization of the black body theorem of electromagnetism, in that it is exponentially insensitive to distant parts of the system. This implies that the projected density of transitions is computationally stable and can be calculated even in macroscopic many-body systems. We argue that the physical content of the density of transitions is determined by the nature of its singular points, such as discrete transitions, continuous spectrum, band edges and van Hove singularities.

1. Extended many-particle systems

The physical properties of macroscopic systems are often strongly influenced by the many-particle interactions among the constituent particles. For example, the rigidity of solids, magnetism and superconductivity are all cooperative many-particle phenomena originating in the correlations between electrons and/or ions in solids. These phenomena are also intrinsically macroscopic in nature, since no finite system exhibits true rigidity, magnetism or superconductivity at any non-zero temperature. Understanding these phenomena thus requires calculations of properties in extended many-particle systems. Unfortunately, for macroscopic systems a full quantum mechanical of treatment of the interactions is rarely possible.

Perhaps the worst of the difficulties encountered in extended many-particle systems are strong coupling and exponential growth in the density of states. The problem of exponential growth is that the number of quantum states in the many-particle Hilbert space grows exponentially with the system size. Not only does the total number of states increase, but with the total density of states at any given energy also increases exponentially, as does the density of states of any given symmetry. The problem of strong coupling is a consequence of this exponential density of states. For any finite strength of the many-particle interaction, there are an exponentially large number of states with energies less than the perturbation strength. Any non-interacting unperturbed state will therefore have

exponentially small overlap with the true interacting particle state, a phenomenon often known as the orthogonality catastrophe. This implies that, in general, perturbation theories will have zero radius of convergence, and useful results can only be obtained by selectively summing infinite classes of diagrams. Many modern methods have been developed to overcome these difficulties, including exact numerical solutions in finite systems using quantum Monte Carlo [1, 2] or exact diagonalization Lanczos [3] methods, renormalization group methods [4, 5], and conserving approximations [6]. While much progress has been made, each of these methods has both advantages and disadvantages, and no single method is adequate to address all the problems of physical interest.

The purpose of this paper is to identify a physical quantity that is computable mathematically and physically stable even in an infinite many-body system. We shall call this quantity the projected density of transitions (or PDOT), denoted by $\rho_Q(\omega)$ where Q is a microscopic operator. For a wide class of many-body models this quantity has the very useful property that it is exponentially *insensitive* to the distant parts of the system or the boundary conditions. The proof of this property is given below, and is essentially an extension of the von Laue black body radiation theorem [7] to the Heisenberg equation of motion. Mathematically, the proof is based on the solution of the classical moment problem [8], which is equivalent to the solution of a wave equation. The PDOT is physically somewhat analogous to the familiar projected density of states (PDOS) of non-interacting systems, and its computation is essentially the natural extension of the recursion method of Haydock and co-workers [9, 10] from non-interacting to many-particle systems. Unfortunately the physical interpretation of the PDOT is less straightforward than for the PDOS. We argue below that the singularities in the spectrum of the PDOT correspond to the thresholds for creating long-lived elementary excitations of the many-body system, and are thus physically meaningful quantities.

The method that we present in this paper has close similarities to the well known Mori formalism, or memory function method, developed in [11–14]. In this method the Liouville superoperator, $L \equiv [H, \ ]$, is used to provide a compact representation of the time evolution of operators under Heisenberg's equation of motion. The Heisenberg equation of motion is transformed into a tridiagonal form, from which a continued fraction expansion is constructed. In our method we also tridiagonalize the Liouville superoperator and construct a continued fraction representation of the spectrum. The principal differences between our method and the Mori approach are in the choice of an inner product for the Hilbert space of operators, and in the physical interpretation of the spectrum. Another important difference is that our main results apply only to the dynamical evolution of *local* or microscopic operators, which we show can be evaluated even in *extended* or macroscopic systems. The black body theorem, which is the central result of this paper, applies only to local operators with our choice of inner product and is not true in the more usual Mori formalism.

The paper is organized into seven further sections. The first of these sets the scene by describing the aspects of the Heisenberg picture that are relevant to what follows, introducing Heisenberg's equation and presenting its formal solution. The next section describes the black body theorem. In section 4 there is a discussion of the representation of operators and the choice of inner product for operators. Section 5 contains our key results, giving a detailed description of the recursive solution of Heisenberg's equation. In section 6 there is a discussion of some simple illustrative examples. Finally, in section 7 we discuss the interpretation of the projected density of transitions for a general interacting system, and section 8 presents some conclusions.

2. The Heisenberg picture

The two conceptual ingredients of quantum mechanics are the states, or wavefunctions, and the observables, or operators, such as velocities and positions. In describing the evolution of a system, the time dependence of physical quantities, which are the expectation values of the observables with respect to the states, can be distributed between the states and the observables in any way. The first important point we make is that for numerical computations in extended many-body systems the Heisenberg picture is considerably more convenient than the Schrödinger picture.

In the Schrödinger picture the time-dependent Schrödinger equation has the familiar formal solution:

$$\psi(t) = \exp(-iHt)\psi(0) \tag{1}$$

(in units in which $\hbar = 1$). The difficulty with this equation in extended many-body systems is that the Hamiltonian $\hat{H}$ is proportional to the system size, and therefore the dominant frequencies contained in a general wavefunction are also proportional to the system size. For example, we can define a formal density of states projected on any state $\psi(0)$:

$$\rho_\psi(E) = \frac{1}{\pi}\Im\left\langle\psi(0)\left|\frac{1}{E - i\epsilon - H}\right|\psi(0)\right\rangle \tag{2}$$

(where ϵ is a positive infinitesimal) but this is not a useful quantity. The reason is that successive moments of this projected density of states grow as powers of the system size, and therefore the projected density of states possesses no well defined moment or continued fraction expansion, in contrast to the single-particle density of states. This is another example of the orthogonality catastrophe, since no finite-energy eigenvector of H, such as the ground state, has any finite overlap with any given trial state $\psi(0)$. The non-existence of the moment expansion for the density of states projected on $\psi(0)$ is also equivalent to the statement that the Taylor series for the time dependence of $\psi(t)$ has zero radius of convergence, since in

$$\psi(t) = [1 - iHt + (-iHt)^2/2 + \ldots]\psi(0) \tag{3}$$

successive terms grow with powers of the system (which might be infinite), and hence the solution in (1) is purely formal in infinite systems. These problems make it necessary to carry out computations only in finite-size systems and then take the thermodynamic limit by finite-size scaling at the end of the calculation.

Now let us contrast this behaviour with the Heisenberg picture. In the Heisenberg picture the time dependence is transferred from the wavefunctions to the operators with the usual time dependence:

$$-i\frac{dQ(t)}{dt} = [H, Q(t)]. \tag{4}$$

Since the above commutation of H with $Q(t)$ is a linear transformation of the operator $Q(t)$, it may be written in terms of a superoperator, L, called the Liouvillian [15]

$$LX \equiv [H, X] \tag{5}$$

for any operator X. The Liouvillian is a superoperator since it is a linear transformation acting on the space of observables or operators rather than on the space of wavefunctions.

If the Hamiltonian is time independent, then the Liouvillian is also time independent and Heisenberg's equation of motion has the formal solution

$$Q(t) = \exp(\mathrm{i}Lt)Q(0). \tag{6}$$

Since Heisenberg's equation is first order its formal solution contains one constant operator, namely $Q(0)$.

This formal solution of Heisenberg's equation shows that the frequencies present in $Q(t)$ are just the eigenvalues or, more precisely, the invariant values of the Liouvillian for the various components of $Q(0)$. The magnitudes of these frequencies can be simply estimated by the growth of $Q(0)$ as it is multiplied by successive powers of the Liouvillian. A little experimentation with different Hamiltonians shows that when Q is a single-particle position, momentum or other variable, these frequencies are characteristic of the binding energies of that particle. When Q involves several particles, its frequency is characteristic of the energy of the several particles. Therefore the characteristic frequencies in (6) are independent of the size of the system, and hence microscopic. This is quite different from the Schrödinger picture, where the characteristic frequencies are proportional to the size of the system and hence macroscopic. We shall prove below that the characteristic frequencies in the Heisenberg picture remain microscopic for a wide range of interesting many-body Hamiltonians, and that this implies that the time evolution of operators possesses a number of useful convergence properties.

3. The black body theorem

Wave equations have the property that the density of modes at one position is exponentially insensitive to distant disturbances. This is called the black body theorem because it explains why black bodies emit a spectrum of electromagnetic radiation that is independent of the black body's shape or material. Even in electromagnetism, this theorem is surprising because, while it is plausible that the spectrum should be insensitive at wavelengths much shorter than the scale of any feature of the black body, different materials do have different optical properties and yet the spectrum is insensitive to this as well. The qualitative explanation is that in thermal equilibrium the spectrum is determined by the normal modes of the cavity, rather than by the nature of the walls. Weyl [16] showed that the total density of modes is independent of the shape of the cavity, provided its dimensions are all much greater than the wavelengths under consideration. Von Laue [7] went on to show that at any point inside the cavity the density of normal modes at a particular frequency depends on the walls to a degree that decreases exponentially with the number of wavelengths (at that frequency) to the nearest wall.

Friedel [17] later argued that the black body theorem also applies to the local density of states of the one-electron Schrödinger equation (see Heine [18] for a commentary on this). In one-electron quantum mechanics, the electronic wavefunctions replace the electromagnetic modes, and the probability density for finding an electron at a given point with a given energy replaces the local density of normal modes. The underlying principle is the same, namely that a change in the material at a distance of several wavelengths affects only the phase, and not the amplitude of the wavefunctions averaged over a small range of energy.

The general form of the black body theorem establishes the local density of modes as a stable physical quantity in systems described by wave equations. The local density of modes at r is given by

$$\rho(r, \omega) = \sum_i |\langle r|\psi_i\rangle|^2 \delta(\omega - \omega_i) \tag{7}$$

where ψ_i is the eigenfunction (whether electromagnetic or Schrödinger) with frequency ω_i. It follows from the properties of the wave equation that the local density of modes averaged over a small range of frequency changes by an amount that decreases exponentially with the distance measured in wavelengths from some disturbance. In contrast, the normal modes themselves are known to be highly sensitive to distant disturbances in the system.

Like Maxwell's and Schrödinger's equations, Heisenberg's equation is an example of a linear wave equation. However, in this case the waves are operators. The normal modes of the Heisenberg equation are the operators with harmonic time dependence

$$Y_a(t) = Y_a \exp(i\omega_a t) \tag{8}$$

where Y_a is an invariant or eigenoperator of the Liouvillian satisfying

$$LY_a = \omega_a Y_a. \tag{9}$$

From the definition of the Liouvillian it is easy to see that its invariant operators, Y_a, have the form of transitions among the different eigenstates of the Hamiltonian:

$$Y_a = |\psi_i\rangle\langle\psi_j| \tag{10}$$

with

$$\omega_a = E_i - E_j \tag{11}$$

where

$$H|\psi_i\rangle = E_i|\psi_i\rangle \tag{12}$$

and the $|\psi_i\rangle$ are the many-body eigenstates of the system with energies E_i.

In order to extend the black body theorem to Heisenberg's equation, the idea of the local density of modes must be generalized to something that describes a local property of the invariant operators in the above equation. To do this we must instead introduce some notion of locality for an operator. We shall call an operator local if it only acts on or changes occupation numbers in a finite region of space. For example, the real-space electron creation and annihilation operators, density operators and so on are familiar local operators. The importance of local operators has also been emphasized by Fulde [19] in a slightly different context.

Secondly, we must resolve a local operator into components at different frequencies. Operators combine linearly, just as waves do, so a component of an operator is a projection of one operator on another. To establish projection among operators we must introduce an inner product, (X, Y), on the space of operators (not to be confused with the inner product of states $\langle\psi|\phi\rangle$). Specific choices of inner products are discussed below in section 4. Given a local operator, say Q, and an inner product $(\,,)$ it is natural to define the following projected density of modes:

$$\rho_Q(\omega) = \sum_a |(Q, Y_a)|^2 \delta(\omega - \omega_a). \tag{13}$$

Since the eigenoperator Y_a is a solution to the wave equation, this projected density of modes is nothing more than the local intensity of each mode. This idea of a projected density of modes is the natural extension of the familiar local density of states of (7). Since the eigenoperators Y_a correspond to transitions among eigenstates, we shall refer to $\rho_Q(\omega)$ as the projected density of transitions (PDOT). It is the central quantity in all the main results of this paper.

The general form of the black body theorem is that the average of the local density of modes over a localized test function is exponentially insensitive to distant disturbances in the system. We shall prove below that the PDOT for Heisenberg's equation obeys the black body theorem, provided that the operator or test function in the projection is localized. The black body theorem then says that any frequency average of the magnitude of the component of the localized operator in each mode is exponentially insensitive to changes in the Liouvillian that are many wavelengths distant. The proof of the black body theorem for Heisenberg's equation follows from the convergence of the continued fraction expansion of the projected density of transitions. The development of this main result is the subject of the next two sections.

4. Inner products and representation of operators

For Heisenberg's equation the black body theorem applies to the projected density of normal modes which requires the definition of an inner product between some localized operator and the normal modes. In other words, we need to define an inner product on the space of operators, (X, Y). This product should obey the usual rules for inner products, such as $(X, Y) = (Y, X)^*$. The most important requirement that the inner product must satisfy is that the Liouvillian superoperator should be Hermitian:

$$(X, LY) = (LX, Y). \tag{14}$$

To see why this is necessary let $Q(0)$ be some localized operator that evolves into $Q(t)$ according to the exponential of the Liouvillian L. The projection of $Q(t)$ onto $Q(0)$ is the inner product $C_Q(t) \equiv (Q(0), Q(t)) = (Q(0), e^{iLt} Q(0))$. If the physical system described by this Liouvillian is invariant under time translations, then the correlation between Q at two different times must also be invariant under time translations, or $(Q(t'), Q(t)) = (e^{iLt'} Q(0), e^{iLt} Q(0)) = C_Q(t - t')$, which is clearly satisfied if L is Hermitian. At least L must be Hermitian in the subspace of operators spanned by $Q(t)$.

The most general inner product for which the Liouvillian is Hermitian is a weighted trace of $X^\dagger$ and Y over eigenstates of the Hamiltonian, i.e.

$$(X, Y) = \sum w_{ij} \langle \psi_i | X^\dagger | \psi_j \rangle \langle \psi_j | Y | \psi_i \rangle \tag{15}$$

where the weights w_{ij} must all be real to fulfill the conjugation condition, $(X, Y) = (Y, X)^*$, but are otherwise arbitrary. This class of inner product leads to a Hermitian Liouvillian, since

$$(LX, Y) = \sum w_{ij} \langle \psi_i | (HX - XH)^\dagger | \psi_j \rangle \langle \psi_j | Y | \psi_i \rangle \tag{16}$$

$$= \sum w_{ij} \langle \psi_i | X^\dagger | \psi_j \rangle \langle \psi_j | (HY - YH) | \psi_i \rangle \tag{17}$$

$$= (X, LY). \tag{18}$$

Within this general form for the inner product there are a variety of possible choices. For example, the Kubo inner product is usually used in the Mori formalism [11, 20]:

$$(X, Y)_K = \frac{1}{\beta} \int_0^\beta d\lambda \langle\langle X^\dagger(-i\lambda) Y(0) \rangle\rangle \tag{19}$$

where $X(-i\lambda)$ is the time-dependent operator analytically continued to the imaginary time axis and $\langle\langle \ \rangle\rangle$ denotes a thermal expectation value at temperature $T = 1/k_B\beta$ in the canonical ensemble. The Kubo inner product has the physical interpretation that it yields the static

change in $\langle\langle X\rangle\rangle$ when the Hamiltonian is perturbed infinitesimally by Y at temperature T [21]. It corresponds to the weight function

$$w_{ij} = \frac{\exp(-\beta E_i) - \exp(-\beta E_j)}{\beta(E_i - E_j)}. \tag{20}$$

Although the Kubo form of the inner product has a number of useful features, it does not allow us to prove the results we are seeking. In particular, there is no black body theorem for the PDOT when the Kubo form is used. The problem is that the thermal expectation values in (19) *do* depend on distant parts of the system. For example, if the system passes through a second-order phase transition the system becomes correlated over arbitrarily long length scales, and thermal expectation values of operators are sensitive to arbitrarily distant perturbations.

Another possible choice of inner product corresponds to the case in which all the states are weighted equally [15, 22]. This inner product could be called the infinite-temperature inner product, since it corresponds to $\beta \to 0$ or constant w_{ij}. This inner product is also known as the trace product, or trace norm, since it becomes simply

$$(X, Y) = \mathrm{Tr}(X^\dagger Y)/\mathrm{Tr}(I) \tag{21}$$

where Tr denotes the trace of a matrix or operator, and I is the identity operator. The normalization factor $1/\mathrm{Tr}(I)$ is not necessary, but is convenient for actual calculations since it ensures $(I, I) = 1$. The trace norm has the important property that if X and Y are local operators only acting in some limited region of space, then the trace norm can be easily computed solely within that region. The trace norm of two local operators is therefore completely insensitive to distant parts of the system, unlike the Kubo inner product.

To give a concrete example, suppose that our system has a basis of localized single-electron Wannier orbitals, atomic spin-orbitals on the sites of a crystal lattice, for example. Let $c_1^\dagger, c_2^\dagger, \ldots$ be electron creation operators that add particles to orbitals $1, 2, \ldots$ etc, and which have the usual anticommutation rules:

$$[c_n^\dagger, c_m]_+ = \delta_{n,m}. \tag{22}$$

Assuming that the Wannier orbitals are orthonormal, it is simple to show that the trace norm inner products of the creation and annihilation operators are

$$(c_n, c_m) = (c_n^\dagger, c_m^\dagger) = \delta_{n,m}/2 \tag{23}$$

$$(c_n^\dagger, c_m) = (c_n, c_m^\dagger) = 0. \tag{24}$$

The operators at site n are orthogonal to the operators at all other sites, and hence the trace norm can be evaluated solely in the region of space containing site n.

The full trace norm is not the only inner product that can be used here. For example, if the trace is restricted to a subspace of the Hamiltonian corresponding to a given symmetry sector, then again a Hermitian Liouvillian is obtained. Trace products with a given particle number or total z-axis spin are also simple to implement. The only absolute requirements we need below are Hermiticity of the Liouvillian and the locality of the inner product of two local operators, and any inner product that satisfies those conditions can be used.

5. Recursive solution of Heisenberg's equation

We are now in a position to derive the central result of this paper, namely the black body theorem for the projected density of transitions. The proof is developed in two stages: first, we show that Heisenberg's equation of motion for a local operator has a Taylor series with a finite radius of convergence; second, we argue that the moment expansion of the PDOT can therefore be represented by a continued fraction expansion. The continued fraction is generated by a straightforward recursion, which is used to prove the black body theorem.

The formal solution of Heisenberg's equation in terms of an exponential of the Liouvillian (6) suggests a power series in time, which may or may not have a finite radius of convergence. For a localized operator $Q(0)$ consider a single component of $Q(t)$, namely its projection back onto $Q(0)$: $(Q(0), Q(t))$. By expanding the exponential of L in a power series, this component can be written as

$$C_Q(t) \equiv (Q(0), Q(t)) = q_0 + iq_1 t - \tfrac{1}{2}q_2 t^2 + \frac{-i}{3!}q_3 t^3 + \ldots + \frac{i^n}{n!}q_n t^n + \ldots \qquad (25)$$

where the coefficients are the moments of L on $Q(0)$:

$$q_n = (Q(0), L^n Q(0)). \qquad (26)$$

For Heisenberg's equation to make sense the above power series must converge, at least for some finite interval of time, however small. From the usual criteria for convergence of a power series, the above expansion for $C_Q(t)$ converges absolutely from time zero to some positive time τ, provided that the moments grow no faster than $n!/\tau^n$. Of course, this does not imply that the time evolution of $Q(t)$ becomes singular at time τ, but just that there is a singularity in the complex t-plane at a distance τ from the origin.

The proof of convergence of the power series in time follows from power counting the moments q_n. Suppose for simplicity that we start with a single creation operator at some lattice site for the initial operator $Q(0)$. Suppose also that each action of L on a creation or annihilation operator produces at most Z new terms. For example, Z will reflect the coordination of the lattice and so on. We also assume that there are only two particle interactions, so that $Lc^\dagger$ can produce strings of no more than three new creation and annihilation operators. We can then see that $LQ(0)$ contains no more than Z terms, each with three or fewer creation or annihilation operators. Now using the operator identity

$$L(XY \ldots Z) = (LX)Y \ldots Z + X(LY) \ldots Z + \ldots + XY \ldots (LZ) \qquad (27)$$

we can see that applying L to $LQ(0)$ we can obtain at most $3Z^2$ terms, which can contain at most five creation or annihilation operators. Repeating this process iteratively we can see that $L^n Q(0)$ contains at most $1.3.5.\ldots.(2n-1)Z^n$ terms containing up to $1.3.5.\ldots.(2n+1)$ creation and annihilation operators. If M is the maximum matrix element for L acting on any single creation or annihilation operator, then the moment q_n cannot exceed $1.3.5.\ldots.(2n-1)(ZM)^n \sim n!(2ZM)^n$. This bound is just sufficient to prove that the Taylor series has a finite radius of convergence, τ, since by the ratio test the series must converge absolutely when $|t| < 1/2ZM$. Note that we are not saying that the power series certainly diverges for $t > 1/2ZM$, but simply that the radius of convergence is at least $1/2ZM$. The radius of convergence may be larger, or even infinite, in some special cases. Clearly the proof can be generalized to any starting operator $Q(0)$ that is a finite combination of creation and annihilation operators, and hence to any localized $Q(0)$ in a fermionic system. For bosons, even a localized operator may contain infinitely long products of creation and annihilation operators, and so it is necessary to make the further restriction

that all such products must be finite. We must also assume that the Hamiltonian does not include any singular or long-ranged potentials, so that the matrix elements remain bounded by M, and Z is finite. This requirement is satisfied by a large number of model many-body Hamiltonians, such as Heisenberg and Hubbard models, but does not allow for long-ranged Coulomb interactions. Singularities in $C_Q(t)$ may arise when $Q(0)$ is delocalized, or when there are singular or long-ranged potentials that give the frequency spectrum of $C_Q(t)$ weight at high frequency. This weight at high frequency means that $C_Q(t)$ goes to zero very rapidly, which is the same thing as saying that the excitation created by $Q(0)$ runs rapidly away to infinity.

The time evolution of the operator $Q(t)$ is most conveniently represented in the frequency domain. The Fourier transformation of Heisenberg's equation is algebraic and its solution is the resolvent of L applied to $Q(0)$ [15]:

$$R(w) = \frac{1}{\omega - L} Q(0). \tag{28}$$

In terms of $R(\omega)$, the solution of the original equation is

$$Q(t) = \frac{1}{2\pi i} \int R(\omega) \exp(i\omega t) d\omega \tag{29}$$

where the integral is taken around a contour in the complex ω-plane that encloses the poles of $1/(\omega - L)$. These poles must lie on the real axis since L has real eigenvalues. The resolvent $R(\omega)$ thus contains the same dynamical information about the time evolution of the operator $Q(t)$ as the original Heisenberg equation. In particular, $R(\omega)$ resolves the operator $Q(t)$ into its component transitions at different frequencies.

The analytic properties of the frequency spectrum are most easily studied by examining a single matrix element of the resolvent, the diagonal $Q(0)$ element of the resolvent:

$$R_Q(\omega) = \left(Q(0), \frac{1}{\omega - L} Q(0) \right) = (Q(0), R(\omega)). \tag{30}$$

This provides a convenient representation of the time evolution of $C_Q(t)$ by the Fourier integral

$$C_Q(t) = \frac{1}{2\pi i} \int R_Q(\omega) \exp(i\omega t) d\omega \tag{31}$$

where again the integration is over a contour that encloses, but does not intersect, the spectrum of the poles of $R_Q(\omega)$ on the real axis. Comparing this representation of $C_Q(t)$ with the Taylor series (25) we see that the moments of the Liouvillian, q_n, are equal to the frequency moments of $R_Q(\omega)$:

$$q_n = \frac{1}{2\pi i} \int R_Q(\omega) \omega^n d\omega. \tag{32}$$

Introducing the *projected density of transitions* (PDOT), $\rho_Q(\omega)$, as the imaginary part of the resolvent for frequencies infinitesimally below the real axis

$$\rho_Q(\omega) = \frac{1}{\pi} \Im R_Q(\omega - i\epsilon) \tag{33}$$

we see that $\rho_Q(\omega)$ is a real and positive function. To see that this corresponds to the original definition of (13) simply evaluate the resolvent (30) on the basis of the invariant operators

of L from (9) and use the usual identity (strictly valid only within an appropriate integral): $\Im 1/(x - i\epsilon) = \pi\delta(x)$. Furthermore, the moments of $\rho_Q(\omega)$ are also given by the q_n:

$$q_n = \int \rho_Q(\omega)\omega^n d\omega \tag{34}$$

where the integration is along the real axis. The bound that the moments grow no faster than $n!(2ZM)^n$ implies that the function $\rho_Q(\omega)$ decays at least exponentially for large ω:

$$\rho_Q(\omega) = O(\exp[-|\omega|/(2ZM)]) \tag{35}$$

as $|\omega| \to \infty$. For a general macroscopic many-body system the spectrum of transitions will not be bounded, since there are transitions among many-body states of all macroscopic energies; however, the exponential decay of the projected density of transitions shows that the spectrum does not behave 'too badly' at infinity, provided the operator $Q(0)$ is local. Using this bound on $\rho_Q(\omega)$ it is clear that (31) converges for all times, t, and can thus be viewed as the analytic continuation of the Taylor series (25) beyond its radius of convergence.

We have now shown that the density of transitions $\rho_Q(\omega)$ projected on a local operator is a positive real function with moments given by the moments of the Liouvillian $q_n \equiv (Q(0), L^n Q(0))$, which can be calculated in a finite number of computational steps. However, the representation of a function in terms of its moments is notoriously ill conditioned. For example, a small error in a moment q_n due to computer rounding error could result in a large change in the value of $\rho_Q(\omega)$ at any specific frequency ω. A much better behaved representation is provided by a continued fraction representation. First we expand the diagonal matrix element of the resolvent:

$$R_Q(\omega) = \frac{q_0}{\omega} + \frac{q_1}{\omega^2} + \frac{q_2}{\omega^3} \cdots \frac{q_n}{\omega^{n+1}} + \cdots . \tag{36}$$

This is now an asymptotic expansion around infinity and seems even less convergent than the power series in time. However, because $R_Q(\omega)$ has all its singularities on the real ω-axis and because they all have positive residues, which follow from conservation of probability by the Hamiltonian, this series can be summed by a continued fraction of the Jacobi type [8]. The continued fraction converges absolutely for all ω off the real axis:

$$R_Q(\omega) = \cfrac{b_0^2}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - \ldots}}} \tag{37}$$

where the parameters of the continued fraction $\{a_n, b_n\}$ are all real, and may be related to the moments by expanding the continued fraction as a power series in $1/\omega$. The continued fraction expansion has the strongest convergence properties of all the series discussed here. In particular, outside its spectrum the continued fraction converges exponentially.

The parameters in the continued fraction expansion $\{a_n, b_n\}$ can calculated from the moments (which is ill conditioned) or by a direct extension of the recursion method [9, 10] to Heisenberg's equation of motion. The original Schrödinger equation recursion method constructs an orthonormal sequence of states $\{u_0, u_1, \ldots, u_n, \ldots\}$ such that the Hamiltonian is successively transformed into a tridiagonal form under the recursion:

$$H u_n = a_n u_n + b_{n+1} u_{n+1} + b_n u_{n-1}. \tag{38}$$

The application of the recursion method to Heisenberg's equation constructs a basis of orthonormal *operators* $\{U_0, U_1, \ldots, U_n, \ldots\}$ in which the Liouvillian *superoperator* is a tridiagonal matrix. In other words, the recursion expresses the Liouvillian as a three-term recurrence:

$$LU_n = a_n U_n + b_{n+1} U_{n+1} + b_n U_{n-1} \qquad n \geqslant 0. \tag{39}$$

This recurrence generates a sequence of operators $\{U_n\}$ which are orthonormal with respect to the inner product:

$$(U_n, U_m) = \delta_{n,m}. \tag{40}$$

The operators U_n are generated by iterating the algorithm

$$a_n = (U_n, LU_n) \tag{41}$$

$$V_{n+1} = LU_n - a_n U_n - b_n U_{n-1} \tag{42}$$

$$b_{n+1}^2 = (V_{n+1}, V_{n+1}) \tag{43}$$

$$U_{n+1} = V_{n+1}/b_{n+1} \tag{44}$$

starting the recurrence with $U_{-1} = 0$ and $U_0 = Q(0)/b_0$, the normalized local operator $Q(0)$ with $b_0^2 = (Q(0), Q(0))$. By construction this recurrence ensures that $(U_n, U_{n+1}) = 0$ and using the fact that L is Hermitian one can prove by induction all the operators $\{U_n\}$ are orthonormal. In the basis of the operators $\{U_n\}$ the Liouvillian superoperator is represented by a symmetric tridiagonal matrix. The matrix $J_{nm} = (U_n, LU_m)$ has the $\{a_n\}$ along the main diagonal and the $\{b_n\}$ along the first upper and lower subdiagonals with the rest of the matrix elements zero. Finally, the resolvent element $(U_0, 1/(\omega - L)U_0)$ can be expressed in the orthonormal basis of the $\{U_n\}$ and corresponds to the leading diagonal element of the inverse of the tridiagonal matrix $\omega I - J$:

$$(U_0, 1/(\omega - L)U_0) = [(\omega I - J)^{-1}]_{00}. \tag{45}$$

This tridiagonal matrix inverse can be computed easily, and corresponds to the continued fraction (37) apart from the trivial normalization constant b_0^2. The coefficients $\{a_n, b_n\}$ generated by the recursion are therefore exactly the same parameters that appear in the continued fraction representation of the resolvent element $R_Q(\omega)$. The resolvent and PDOT can therefore be computed directly by the recursion (44). All of these results are simply equivalent to the usual recursion method results [10], except that the orthonormal states u_n are replaced by the orthonormal operators U_n and the Hamiltonian operator is replaced by the Liouvillian superoperator.

The above paragraphs complete the derivation of the main results of this paper, so let us now summarize and discuss the implications of these results. The result has been to show that, starting from a local operator $Q(0)$, it is possible to tridiagonalize the Liouvillian superoperator. The tridiagonalization gives the coefficients in the continued fraction expansion of the projected resolvent $R_Q(\omega)$. The continued fraction converges absolutely and exponentially for all ω off the real axis, because it corresponds to a well defined moment expansion. The bounds on the moments ensures that the PDOT $\rho_Q(\omega)$ has at least an exponentially decaying spectrum at large frequencies. The existence of the Liouvillian tridiagonalization has been known since the work of Mori [11]; however, the proof of its convergence relies explicitly on the locality of the operators and inner product and has not been given before to our knowledge.

We are now, finally, in a position to demonstrate the important physical result that the PDOT $\rho_Q(\omega)$ is exponentially insensitive to distant parts of the system, i.e. that it obeys the black body theorem. The proof is very straightforward using the machinery we have assembled above. We have already said that at any ω off the real axis the continued fraction expansion of $R_Q(\omega)$ converges exponentially. This means that the changes in $R_Q(\omega)$ induced by perturbing or truncating the continued fraction at the nth level decrease exponentially as n increases. Now, the coefficients of the nth level of the continued fraction are obtained from the operators U_n and U_{n-1}, which are in turn linear combinations of $Q(0)$, $LQ(0)$, ..., $L^n Q(0)$. But if there are no long-ranged interactions or hopping terms in the Hamiltonian, then these operators are local and will only act within a finite radius (of order n) of the region where the initial local operator $Q(0)$ acts. The continued fraction up to order n is thus *completely insensitive* to the system beyond this radius. Therefore $R_Q(\omega)$ slightly off the real axis is exponentially insensitive to distant parts of the system. Finally, since the PDOT $\rho_Q(\omega)$ is simply the imaginary part of $R_Q(\omega)$ evaluated slightly off the real axis it too is completely insensitive to distant parts of the system. Alternatively, by a Hilbert transform

$$R_Q(\omega) = \frac{1}{\pi} \int d\omega' \frac{\rho_Q(\omega')}{\omega - \omega'} \tag{46}$$

integrating along the real axis, $R_Q(\omega)$ slightly off the real axis, say with imaginary part ϵ, depends on a Lorentzian weighted integral of $\rho_Q(\omega)$ over a range of frequencies of width ϵ. Therefore, if $R_Q(\omega)$ is exponentially insensitive to the distant parts of the system, then integrals of $\rho_Q(\omega)$ over small regions must also converge. This completes the proof of the black body theorem for the Heisenberg equation. Notice that $\rho_Q(\omega)$ converges *in quadrature*, but not necessarily point by point on the frequency axis; this is exactly the same as the black body convergence for electromagnetic or Schrödinger wave equations [23].

6. Examples

6.1. Non-interacting electrons

As a first simple example of the Liouvillian recursion method we shall show that for non-interacting electron systems the method becomes identical to the ordinary recursion method [9, 10]. Consider the electronic Hamiltonian

$$H = \sum H_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \tag{47}$$

where $c_{i\sigma}^{\dagger}$ and $c_{j\sigma}$ create and annihilate spin-σ electrons in local orbitals i and j respectively. H_{ij} is a single-particle Hamiltonian, which contains diagonal site energies and off-diagonal hopping terms.

We choose a starting operator for the recursion that adds a particle at some site, say 0: $U_0 = \sqrt{2} c_{0\uparrow}^{\dagger}$. The factor of $\sqrt{2}$ is chosen to ensure the normalization $(U_0, U_0) = 1$ using the fermion operator inner products given above in (24). It is simple to see from the fermion commutation rules that

$$L c_{0\uparrow}^{\dagger} = \sum H_{i0} c_{i\uparrow}^{\dagger} \tag{48}$$

and therefore the action of the Liouvillian is to move the electron to neighbouring sites. Similarly, after n actions of the Liouvillian:

$$L^n c_{0\uparrow}^{\dagger} = \sum H_{ij} H_{jk} \ldots H_{m0} c_{i\uparrow}^{\dagger}. \tag{49}$$

Using the trace norm inner product defined above we find the moments:

$$(U_0, L^n U_0) = \sum H_{0j} H_{jk} \dots H_{m0} = [H^n]_{00} \tag{50}$$

identical to the Hamiltonian moments. It is clear from this example that the Liouvillian continued fraction coefficients $\{a_n, b_n\}$ are identical to the ordinary recursion method continued fraction coefficients that would have been obtained by recursion with the Hamiltonian matrix acting on a normalized state, u_0 at site 0.

This result implies that for non-interacting systems the Liouvillian recursion starting with a single creation operator becomes identical to the conventional Hamiltonian recursion. The PDOT therefore becomes identical to the ordinary single-particle density of states projected onto orbital 0 and spin up. This provides a simple example, which will aid in interpreting the physical meaning of the PDOT. The PDOT is a weighted density of transitions among many-body eigenstates. In the case when U_0 is a single-particle creation operator these are transitions between the spaces of many-body states of N and $N + 1$ particles. The PDOT picks out the density of these transitions at each frequency, which for non-interacting systems is just the single-particle projected density of states.

A related example, which shows how the Liouville recursion method goes beyond the usual Hamiltonian formulation, is the Bogolibov–de Gennes Hamiltonian of a superconductor:

$$H = \sum H_{ij\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \Delta_{ij} c^{\dagger}_{i\sigma} c^{\dagger}_{j-\sigma} + \Delta^*_{ij} c_{j-\sigma} c_{i\sigma}. \tag{51}$$

The many-body eigenstates of this Hamiltonian are subtle since they do not have a definite particle number because of the non-zero gap function Δ_{ij}. However, the Hamiltonian can be diagonalized straightforwardly by Bogolibov transformation. Using the Liouville recursion exactly as outlined above, and a starting operator such as $U_0 = \sqrt{2} c^{\dagger}_{0\uparrow}$, one immediately computes the spectrum of the Bogolibov quasiparticles [24]. Since these quasiparticles are non-interacting the PDOT is again equivalent to the projected density of states. However, in this case the transitions that diagonalize the Liouvillian are linear combinations of $c^{\dagger}$ and c operators. Hence they are not transitions between many-body states of definite particle numbers, but are transitions that create or destroy Bogolibov quasiparticles.

6.2. Finite systems

Another simple but instructive example is provided by systems for which the many-body Hilbert space has finite dimension. For example, the finite-size clusters of Hubbard or Heisenberg model many-body systems that are studied with exact diagonalization techniques fall into this category [3]. For a system with a finite-dimensional Hilbert space we can simply enumerate the set of basis states, say $|\psi_i\rangle$, for $i = 1, N$. The Hamiltonian and other operators are just finite $N \times N$ matrices. With any normalized starting matrix U_0 we may use the Liouvillian recursion to generate a sequence of orthonormal matrices, U_1, U_2, etc. Since there are at most N^2 possible orthonormal matrices the recursion must terminate ($b_n = 0$) after a finite number of steps (ignoring numerical rounding errors). The continued fraction for this system is thus finite, corresponding to a PDOT $\rho_Q(\omega)$ given by a set of up to N^2 delta functions:

$$\rho_Q(\omega) = \sum_a w_a \delta(\omega - \omega_a). \tag{52}$$

Again the interpretation of this result is clear. For a finite system there are N many-particle eigenstates with energies E_i, and thus a total of N^2 possible transitions with frequencies $\omega_a = E_i - E_j$. Whatever starting operator, U_0, or inner product $(,)$ are chosen the PDOT will correspond to a weighted sum of these different transition frequencies. Different starting operators or inner products can merely change the weights of the various transitions, w_a.

6.3. Heisenberg and Hubbard models

Since it is explicitly local the Liouvillian recursion can be easily carried out in lattice models, such as the quantum Heisenberg or Hubbard models. These models are especially important cases since conventional methods, such as many-body perturbation theory, are generally not useful because of strong coupling.

For example, in the Heisenberg model

$$H = J \sum_{\langle ij \rangle} S_i \cdot S_j \tag{53}$$

there are $(2S + 1)^2$ possible operators for each lattice site. For the case of spin $\frac{1}{2}$ there are four, conveniently chosen as the identity, I, and the Pauli matrices σ_i. It is readily verified that these are an orthonormal set under the trace norm [22]. A general operator is a linear combination of products of these four basis operators. By definition a local operator is one that differs from the identity only within a finite region of space. Equivalently, it is one that is a non-identity at only a finite number of sites. Clearly, if Q is a local operator, the LQ is also local since the Hamiltonian only connects neighbouring sites.

For a specific example, consider taking a normalized starting operator at the origin, $U_0 = \sigma_{0z}$, we obtain:

$$[H, \sigma_{0z}] = \frac{J}{4} \sum_{\langle i0 \rangle} (-2i\sigma_{ix}\sigma_{0y} + 2i\sigma_{iy}\sigma_{0x}) \tag{54}$$

and hence $a_1 = 0$, $b_1 = J\sqrt{Z/2}$ and

$$U_1 = \frac{1}{\sqrt{2Z}} \sum_{\langle i0 \rangle} (-i\sigma_{ix}\sigma_{0y} + i\sigma_{iy}\sigma_{0x}) \tag{55}$$

where Z is the lattice coordination number. Notice that a_1 and b_1 are completely insensitive to the dimensionality of space or other details of the lattice topology except its coordination number, an example of the extreme locality of the Liouvillian recursion. The iteration is readily repeated by hand for a few terms, or on a computer for several more continued fraction levels. For example, analytic solutions to some related spin models have been derived by Florencio and co-workers [25, 26], while high-order moments have been derived numerically for the one-dimensional Heisenberg model [27, 28].

Similarly for the Hubbard model

$$H = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{56}$$

there are sixteen basis operators per site composed of products of $\sqrt{2}c_\sigma^\dagger$, $\sqrt{2}c_\sigma$, I and $(I - 2n_\sigma)$ for each spin. Again these are orthonormal under the trace norm. Starting with a single creation operator at the origin, $U_0 = \sqrt{2}c_{0\uparrow}^\dagger$, we obtain

$$[H, U_0] = -\sqrt{2}t \sum_{\langle 0i \rangle} c_{i\uparrow}^\dagger + \sqrt{2}U c_{0\uparrow}^\dagger n_{0\downarrow} \tag{57}$$

and $a_1 = U/2$

$$b_1 U_1 = -\sqrt{2}t \sum_{\langle 0i \rangle} c_{i\uparrow}^\dagger + \sqrt{2}U/2 c_{0\uparrow}^\dagger (2n_{0\downarrow} - 1) \tag{58}$$

and $b_1^2 = Zt^2 + U^2/4$.

For both Heisenberg and Hubbard models the recursion can be carried out numerically until the number of operators in a given U_n fill the available computer storage. For example, on a computer the basis operators for the Heisenberg model can be represented as integers in base 4, where the ith digit represents the four possible operators at site i. The Heisenberg model commutators act to simply flip bits in these integers. As successive commutators are computed the number of operators that must be retained grows exponentially. The number of terms that can be obtained exactly depends on the Hamiltonian and lattice coordination. Making use of efficient storage schemes the typical limit is about 10^7 terms on modern computers. For the one-dimensional Heisenberg Hamiltonians this limit is reached at the 15th recursion level (or 30th moment) [27].

Beyond this computational limit there are a number of possible courses of action. (i) It is often possible extrapolate the recursion coefficients $\{a_n, b_n\}$ by estimating their asymptotic behaviour, or making use of exact asymptotic properties where they are known. This amounts to choosing an appropriate terminating function for the continued fraction [29]. (ii) It may be possible to solve a related model, H_0, analytically (for example the x–y spin model [25] or $U = 0$ Hubbard model are analytic) and then use recursion perturbation theory to extract the recursion coefficients of $H_0 + \lambda V$ in powers of λ [10]. This method proved very powerful in the recursion theory of Anderson localization [30]. (iii) It is possible to numerically truncate the number of terms that are retained during each iteration, which is called dynamic recursion. Because of the exponential insensitivity of the PDOT to distant perturbations such truncation errors are relatively unimportant for practical purposes, just as numerical rounding error does not degrade the projected density of states in the ordinary recursion method [31].

7. Interpretation of the projected density of transitions

The above discussion shows that the projected density of transitions (PDOT) is stable with respect to changes in distant parts of the system and that it can be calculated recursively by tridiagonalizing the Liouvillian in a basis of orthonormal operators. It remains to show how the physical properties of the system may be extracted from this calculation.

One simple interpretation of the PDOT is that it corresponds to a thermodynamic dynamical correlation function, evaluated in an infinite-temperature ensemble. It has been known since the work of Mori [11] that time-dependent correlation functions have continued fraction representations that can be generated recursively. The inner product that must be used is the Kubo inner product at temperature T discussed above. However, the Kubo norm becomes identical to the trace norm as the temperature becomes infinite, and thus the PDOT can be interpreted as a time-dependent correlation function in an infinite-temperature canonical ensemble. This correspondence of the PDOT with infinite-temperature dynamics can be seen clearly by representing the PDOT explicitly in terms of the many-body eigenstates:

$$\rho_Q(\omega) = \sum_{ij} |\langle \psi_i | Q | \psi_j \rangle|^2 \delta(\omega - E_i + E_j). \tag{59}$$

A finite-temperature correlation function would require additional Boltzmann factors of $e^{-\beta E_i}$ in the sum, as occur when the Kubo inner product is used. Since finite-temperature Kubo products are difficult to compute, thermodynamic correlation functions are much more difficult to obtain than the PDOT except in the infinite-temperature limit [25–28].

On the other hand, it seems to us that the PDOT has a wider physical significance than just describing dynamics of infinite-temperature systems. The PDOT contains a weighted sum of

all the possible transitions in the many-body system, and therefore it contains information about all of the eigenstates and energy differences of the Hamiltonian. The difficulty is in extracting this information from the PDOT, since the eigenvalues and eigenstates of the Hamiltonian are macroscopic quantities, which cannot easily be determined from purely local microscopic information such as the PDOT. However, in principle the Liouvillian recursion we have carried out does indeed contain a great deal of physical information about the system, since it contains a complete solution of Heisenberg's equation of motion for any given local starting operator. Furthermore, this solution did not assume any particular temperature, or even a thermodynamic ensemble of any kind. The choice of inner product was merely a mathematical convenience and did not imply any physical choices about thermodynamics. Using the trace norm inner product we achieve a representation of the time evolution of the starting operator

$$Q(t) = \frac{1}{2\pi i} \int 1/(\omega - L)Q(0)\exp(i\omega t)d\omega = \frac{b_0}{2\pi i} \int [(\omega - J)^{-1}]_{0n}U_n\exp(i\omega t)d\omega \qquad (60)$$

in terms of J, the tridiagonal matrix representation for L. Furthermore, although the specific basis of operators U_n which tridiagonalize L and the continued fraction parameters $\{a_n, b_n\}$ depend on the choice of inner product, the time-dependent operator $Q(t)$ is independent of the basis operators and matrix representation of L. Different choices of inner product amount to linear transformations among the orthonormal basis operators which must leave $Q(t)$ invariant. The choice of inner product therefore has no direct physical significance. The physics enters in evaluating expectation values of the time-dependent operator $Q(t)$, which can be obtained in any quantum state or set of quantum states desired, whether zero temperature, finite temperature, infinite temperature or with any arbitrary non-equilibrium density matrix.

Given that the choice of inner product has no physical significance the question arises as to whether the PDOT itself has any physical significance. We believe that the PDOT does indeed contain important physical information about the system, and is therefore a useful quantity to compute. We have three arguments for the direct physical significance of the PDOT.

The first argument that the projected density of transitions contains physical information independent of the thermodynamic ensemble or temperature comes from the results for non-interacting systems. As we showed above, for non-interacting electron systems the PDOT for a single-particle creation operator becomes precisely the projected density of states (PDOS) for the corresponding local orbital. The PDOS is purely a property of the Hamiltonian, and independent of the temperature of the system. If instead of the trace norm we had used the Kubo inner product at temperature T, we would have obtained not the PDOS but the time-dependent thermodynamic Green function for the electrons, which is a function of both temperature and chemical potential. The PDOT computed with the trace norm can therefore have a quite different physical meaning from the quantities computed in the Mori formalism.

The second argument that physical information can be directly extracted from the PDOT comes from considering finite-size systems. We have already shown that for these systems the PDOT converges to a weighted set of delta functions, at each eigenvalue difference of the system: $\omega_a = E_i - E_j$. We can also evaluate the eigenoperator of the Liouvillian, $LY_a = \omega_a Y_a$, for this frequency, since it is just given in terms of the tridiagonalization:

$$Y_a = \sum_n P_n(\omega_a)U_n. \qquad (61)$$

Here $P_n(\omega)$ are the orthogonal polynomials corresponding to the continued fraction $\{a_n, b_n\}$ [10]. But, as mentioned in the introduction, the eigenoperators of the Liouvillian

correspond to direct transitions between eigenstates:

$$Y_a = |i\rangle\langle j| \tag{62}$$

provided that the Liouvillian spectrum has no degeneracies. Thus, by tridiagonalizing the Liouvillian in a finite system, one can in principle directly construct the eigenvalues and operators which project onto specific eigenstates of the Hamiltonian. Clearly, the full spectrum of the Hamiltonian is thus determined from the Liouvillian recursion. Notice, again, that these statements are completely independent of the temperature of the system; we have constructed the full spectrum independent of any choice of thermodynamic ensemble.

The third, and most subtle, argument for direct physical significance is that in the macroscopic limit the positions and natures of singularities in the PDOT are independent of the choice of inner product and of the local operator which initiates the recursion. Consider first what happens to the PDOT as the system size increases toward the macroscopic limit. At any finite size the PDOT consists of isolated delta functions at discrete transition frequencies. As the system size increases the number of transitions grows exponentially, and their spacing decreases exponentially. In the macroscopic limit the continued fraction representation of the PDOT allows several distinct possibilities for the spectrum $\rho_Q(\omega)$: it may still contain isolated delta functions; it may contain dense sets of delta functions (discrete pointwise spectrum); it may contain a singular continuous spectrum where the PDOT is infinite but the infinities contain no weight and it may contain absolute continua where $\rho_Q(\omega)$ is continuous and finite. In general there will also be band edges separating the absolute continua from other spectral regions or gaps with $\rho_Q(\omega) = 0$. Finally, the absolute continua can contain frequencies where the PDOT or one of its derivatives is discontinuous (called van Hove singularities in band theory). The positions and natures of the singularities in the spectrum are determined exactly by the asymptotic behaviour of the continued fraction coefficients $\{a_n, b_n\}$ [32], just as they are determined by the macroscopic limit of finite systems. Since for finite systems the choice of inner product and starting operator only affects the weights of the delta functions, and provided the inner product is not singular itself, then it follows that the positions and natures of the singularities are not affected by either the inner product or the starting operator. Band edges in the PDOT correspond physically to thresholds for excitation which, by the preceding argument, are independent of the inner product or starting operator.

Singularities in the PDOT spectrum are important physically since they correspond to the longest-lived contributions to $C_Q(t)$. This follows simply from (31), which shows that $C_Q(t)$ is the Fourier transform of the PDOT. In most cases excitations $Q(0)$ created at time $t = 0$ soon run away to infinity and so $C_Q(t) = (Q(0), Q(t))$ falls rapidly to zero as t increases. Discrete delta functions in the spectrum correspond to infinitely long-lived contributions, however, and hence to excitations $Q(t)$ that remain in the region of the solid where they were created. Band edges correspond to contributions with power law time decay, while excitations within the absolute continua correspond to exponentially decaying contributions to $C_Q(t)$.

In fact, we can go further and construct operators corresponding to the excitations at the frequencies where the PDOT is singular. These operators have the physical significance that they create long-lived slowly moving excitations, i.e. localized or band edge elementary excitations of the system. If ω_c is the singular frequency, then the corresponding excitation operator is

$$Y_c = \sum_n P_n(\omega_c) U_n \tag{63}$$

where again $P_n(\omega)$ are orthogonal polynomials generated by the continued fraction. If ω_c is an isolated delta function then the $P_n(\omega_c)$ decrease exponentially with n, and this is an absolutely convergent series. The operator Y_c to which the series converges is necessarily a projection between two exact eigenstates of the many-body system: $|i\rangle\langle j|$, provided the transition is non-degenerate. If the singular frequency ω_c is a band edge or a van Hove singularity inside an absolutely continuous region then the construction of the corresponding operator is less straightforward since the convergence is weaker. However, by truncating the series after n terms one obtains an approximation to the transition operator which creates excitations close to the singular frequency. Increasing n produces an operator that is closer to the true singular transition operator, but that is increasingly spread out spatially. This behaviour is familiar from considerations of band edge states in non-interacting electronic systems: since the state precisely at the band edge is extended it cannot be obtained by any finite sum of local states. However at any finite sum of terms one obtains a state that approximates the band edge state over a finite region of space and within some finite-energy resolution of the true band edge. These considerations apply equally to interacting and non-interacting systems.

These critical excitation operators also have the important property that they allow us to obtain convergent expressions for expectation values. In general, the Liouvillian recursion only contains information about energy differences and so cannot be used to construct many-body states of a given energy or to obtain many-body expectation values. The exceptions to this rule are frequencies when the invariant operator

$$Y_c = \sum_n P_n(\omega_c) U_n \tag{64}$$

converges to a *unique* transition $|i\rangle\langle j|$ between exact eigenstates. Then Y_c is a projection operator onto a specific many-body eigenstate and for any operator O (not necessarily one of the recursion operators) and we obtain

$$\langle i|O|i\rangle = \frac{\mathrm{Tr}(Y_c^\dagger O Y_c)}{\mathrm{Tr}(Y_c^\dagger Y_c)} = \frac{(Y_c, O Y_c)}{(Y_c, Y_c)} \tag{65}$$

and

$$\langle j|O|j\rangle = \frac{\mathrm{Tr}(Y_c O Y_c^\dagger)}{\mathrm{Tr}(Y_c Y_c^\dagger)} = \frac{(Y_c^\dagger, O Y_c^\dagger)}{(Y_c^\dagger, Y_c^\dagger)}. \tag{66}$$

Provided the series (64) converges to the unique transition then these expectation values also must converge. For finite systems with a non-degenerate Liouvillian these formulae must converge in a finite number of terms. Similarly isolated transitions in an extended system correspond to unique initial and final states to which the operator Y_c converges exponentially. The expectation values of those states therefore must also converge. Similarly a band edge or van Hove singularity in the PDOT will also correspond to unique initial and final many-body states. For example, the band gap in a semiconductor corresponds to a hole quasiparticle in the state at the top of the valence band and an electron quasiparticle in the state at the bottom of the conduction band. Similarly in spin models with a gap, such as the $S = 1$ spin chain [33], there will be a threshold for transitions from the (unique) ground state to the first excited state. Provided that the first excited state is non-degenerate (or the first excited state of a given symmetry is) then there will be a unique threshold transition and we can construct the threshold operators and the initial- and final-state expectation values. The only caveat is that the critical transition must have a finite weight in the spectrum of the PDOT.

8. Numerical and analytic applications

We have presented the natural generalization of the recursion method of Haydock and co-workers to interacting systems. We have shown that the Liouville superoperator may be recursively transformed into a tridiagonal form on a basis of localized orthonormal operators. The transformation allows us to completely solve Heisenberg's equation of motion for a localized operator. The Taylor series expansion of the time evolution has a finite radius of convergence and a well defined moment expansion exists, which corresponds to a convergent continued fraction. These results contrast with the time dependence of the many-body wavefunctions, where no well defined moment expansion exists for extended systems.

We have shown that there exists an important physical quantity, $\rho_Q(\omega)$, which has the property that it is exponentially insensitive to the distant parts of the system. In other words the spectrum $\rho_Q(\omega)$ obeys a generalization of the black body theorem of von Laue. We call this quantity the projected density of transitions (PDOT) since it is a sum of all the possible transitions from initial to final many-body states weighted by their components on a given local operator. The physical interpretation of the PDOT is rather subtle, but for non-interacting systems it becomes the same as the projected density of states. In particular, the singularities of the spectrum of $\rho_Q(\omega)$ correspond to the long-lived and slow-moving elementary excitations.

Additionally, we have pointed out that the invariant operators of the Liouvillian can be expanded in products of the orthogonal polynomials for the PDOT with the operators which tridiagonalize the Liouvillian. For critical transitions with unique initial and final states these invariant operators consist of a transition operator between two stationary states of the system. Expectation values in the initial or final state can be obtained by taking the trace of the product of an observable with the invariant operator. The analogous expansion of invariant states in products of orthogonal polynomials for the PDOS has been used for non-interacting systems to obtain asymptotic properties such as localization [30].

Our formalism has very close similarities to the Mori formalism [11], but has some crucial differences. The Mori formalism gives continued fraction representations of dynamical correlation functions among operators as a function of temperature, chemical potential and so on. In contrast, the PDOT does not correspond to any particular choice of temperature, or even a thermodynamic ensemble at all, but merely weights all possible transitions which can occur in a given quantum system. This difference is most noticeable in the different inner products used in the two formalisms: the Kubo inner product in the Mori method compared to the trace norm used here. Although the trace norm can be viewed as an infinite-temperature limit of the Kubo inner product, our interpretation of the PDOT is quite different from a thermal correlation function. In our interpretation the trace norm does not have direct physical significance, but is important mathematically in ensuring that the PDOT obeys the black body theorem. Another difference is the key emphasis placed on the locality of the operators in our method, which is not an important consideration in the Mori formalism. Our proofs of convergence of the continued fraction for local operators and the black body theorem for the PDOT are also new as far as we know.

A great deal is already known from non-interacting models about possible behaviours of the continued fraction expansions and projected density of states [32]. All of these earlier results can be taken over without change to the interacting case, once it is clear that the PDOT obeys the back body theorem. Additionally, many numerical calculations already exist using essentially the same formalism we have presented here. These earlier calculations interpreted their results as corresponding to time-dependent correlations in the

Mori formalism at infinite-temperature. In our interpretation, these previous results have obtained the PDOT, which is an intrinsic property of the transitions in the system and not specifically an infinite-temperature quantity. For example, in the one-dimensional XY and transverse Ising models the continued fraction parameters are known to all levels, and thus the complete PDOT is known [25, 26]. In more complex systems, such as the one-dimensional Heisenberg model, the continued fraction parameters must be computed numerically. In the 1D Heisenberg model 30 'infinite-temperature' moments are known, equivalent to a 15-level continued fraction [28]. Unfortunately a continued fraction of this length is usually insufficient to reliably identify critical frequencies unless it becomes clear how to extrapolate the continued fraction parameters. Also, for many of the important many-body Hamiltonians, such as Hubbard and Heisenberg models, it will probably only be possible to obtain a few continued fraction levels, since the number of operators generated by repeated commutation with the Hamiltonian grows exponentially fast.

Recent developments in understanding the effects of numerical errors on the recursion method [23] indicate that the computational approach can be extended far beyond what has been done. Although the number of operators generated by the recursion can grow as fast as a factorial, the errors generated by neglecting small components in the tridiagonal basis for the Liouvillian do not accumulate. This means that, despite this rapid growth, interacting Liouvillians can be tridiagonalized to far greater depth than previously thought, and the resulting continued fractions should give a much more accurate PDOT. From Paige's theorem for the accuracy of Lanczos eigenvectors [34] it follows that the orthogonal polynomial expansion for the invariant operators is also insensitive to the neglect of small components during the tridiagonalization.

In general, our method lacks a direct approach for determining ground-state or thermodynamic information about a given system. The exception is when a transition corresponds to unique initial and final states, such as in a non-degenerate finite system, or as a band edge or excitation threshold in an extended system. Somehow it would appear that in general ground-state information should indeed be contained in this formalism, since we have obtained a complete solution to Heisenberg's equation of motion. One possibility that we have explored is to construct 'lowering' operators, which are operators that lower the energy of any state they act on. Presumably these operators should yield projection operators that can project a given trial wavefunction onto the ground state. Such a lowering operator is easily constructed from the orthonormal basis operators:

$$X^- = \int_{-\infty}^{0} d\omega A(\omega) \sum_n P_n(\omega) U_n \tag{67}$$

where $A(\omega)$ is any arbitrary function. It is also possible to construct perturbation theories in which a non-interacting model Liouvillian L_0 is first tridiagonalized and then the interactions V are introduced perturbatively. The perturbation theory for the resulting continued fraction is identical to the conventional recursion method perturbation theory [10]. However, such topics are perhaps best left for a future paper.

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