A Renormalisation-Group Algorithm for Eigenvalue Density Functions of Interacting Quantum Systems

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We present a certifiable algorithm to calculate the eigenvalue density function — the number of eigenvalues within an infinitesimal interval — for an arbitrary 1D interacting quantum spin system. Our method provides an arbitrarily accurate numerical representation for the smeared eigenvalue density function, which is the convolution of the eigenvalue density function with a gaussian of prespecified width. In addition, with our algorithm it is possible to investigate the density of states near the ground state. This can be used to numerically determine the size of the ground-state energy gap for the system to within a prespecified confidence interval. Our method exploits a finitely correlated state/matrix product state representation of the propagator and applies equally to disordered and critical interacting 1D quantum spin systems. We illustrate our method by calculating an approximation to the eigenvalue density function for a random antiferromagnetic Heisenberg model.

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The statics and dynamics of interacting quantum many-particle systems are still relatively poorly understood. Indeed, even calculating an approximation to such basic quantities as the ground-state energy appears to be extremely difficult for many interesting systems. At least one reason for this is that for arbitrary local quantum systems this problem is complete for the complexity class QMA, which is the quantum analogue of NP [1, 2, 3]. Of course, we do not really expect that there exist general efficient computational schemes to study eigenvalues and related thermodynamic properties. But, it is plausible that for realistic quantum systems there may exist efficient schemes to calculate certain physical properties like approximations to energy gaps and other thermodynamic properties.

The development of the density matrix renormalisation group (DMRG) has provided us with what promises to be an efficient way to calculate physical properties of the ground states of interacting quantum systems in 1D (see [4] and references therein for a detailed description of the DMRG). While the method was originally developed to obtain approximations to the ground state of a regular interacting quantum spin lattice system in 1D, the DMRG is an extremely flexible method and has been recently extended to apply to a diverse number of situations, such as the calculation of short-time dynamics [5, 6], dissipation [7, 8], eigenstates with definite momentum [9], and, recently, higher dimensions [10].

Whether the DMRG and related algorithms actually compute approximations to the ground state of a quantum system instead of low-lying excited states is an open question. This problem is difficult to answer because the DMRG cannot be certified, i.e., once the DMRG produces a ground-state approximation there is no way to prove that this approximation is correct to within some prespecified confidence interval. However, this situation is changing; there have recently been several works which provide certifiable DMRG-like algorithms to approximate ground states of interacting spin systems [11, 12, 13, 14, 15, 16, 17].

One situation where DMRG-related algorithms have been less successful is in the calculation of the eigenvalue density function \( \mu_H(x) \) and the eigenvalue counting function \( N_H(x) \), which counts the number of eigenvalues of a hamiltonian \( H \) with value less than \( x \) [21]. (The two functions are connected by \( \mu_H(x) = dN_H(x)/dx \).) Perhaps the closest general method which has been developed along these lines is due to Porras, Verstraete, and Cirac [9]. This method calculates eigenstates with definite linear momentum for 1D quantum spin systems on a ring. However, it is possible for the method of Porras, Verstrate, and Cirac to miss eigenstates in the same way that the DMRG can miss the ground state and end up in a local minima. While this never appears to occur in practice it would be desirable to have a method which trades this uncertainty against some other approximation. Additionally, if the method of Porras, Verstraete, and Cirac is used to calculate \( \mu_H(x) \) for \( x \gg O(1) \) above the ground state energy then this would require exponential resources.

In this Letter we introduce a certifiable method to calculate systematic approximations to \( \mu_H(x) \) for rather general 1D quantum spin systems (a generalisation to two and higher dimensions is available, which uses a slight modification of the technology of Verstraete and Cirac [10] and [18]). We assume neither translation invariance nor non-criticality. Our method is an approximation because it calculates a “smeared” version \( \tilde{\mu}_H(x) \) of \( \mu_H(x) \), which is the convolution of \( \mu_H(x) \) with a gaussian which has a width which can be reduced with a complexity that provably scales polynomially with \( n \). Our method doesn’t suffer from the uncertainty of the method of Porras, Verstraete, and Cirac, i.e., that maybe some eigenstates are missed. However, the price we pay for this is that while it is certain that every eigenvalue is represented in \( \tilde{\mu}_H(x) \) there is some inevitable uncertainty in the calculated positions of the eigenvalues.
The outline of this Letter is as follows. We begin by introducing some definitions and we introduce the class of systems we study. We then describe our numerical renormalisation group method to calculate $\mu_H(x)$. We conclude with some numerical results of our method applied to a random antiferromagnetic Heisenberg model.

We will, for the sake of clarity, introduce and describe our method for a chain of $n$ distinguishable spin-$\frac{1}{2}$ particles. Thus, the Hilbert space $\mathcal{H}$ for our system is given by $\mathcal{H} = \bigotimes_{j=0}^{n-1} C^2$. Consider the $C^*$-algebra $B(\mathcal{H})$ which is the Hilbert space of all (bounded) linear operators $A$ on $\mathcal{H}$ with inner product $(A,B) = \text{tr}(A^\dagger B)$. An orthonormal basis of $B(\mathcal{H})$ is given by $\sigma^\alpha = \sigma^{\alpha_0} \otimes \sigma^{\alpha_1} \otimes \ldots \sigma^{\alpha_{n-1}}$, $\alpha_j \in \mathbb{Z}/4\mathbb{Z}$, $0 \leq j \leq n-1$, which we call the standard operator basis, where $\sigma^\alpha = [(\frac{1}{\sqrt{2}} \frac{i}{\sqrt{2}}), (\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}}), (\frac{-1}{\sqrt{2}} \frac{i}{\sqrt{2}}), (\frac{-1}{\sqrt{2}} \frac{-i}{\sqrt{2}})]$, is the vector of Pauli sigma matrices. We write the structure constants $g^{\alpha \beta \gamma}$ for the $C^*$-algebra generated by $\sigma^\alpha$: $\sigma^\alpha \sigma^\beta = \sum_\gamma g^{\alpha \beta \gamma} \sigma^\gamma$. The family $H$ of local hamiltonians we focus on is defined by $H = \sum_{j=0}^{n-1} h_j$, where $h_j$ is an interaction term which couples only neighbouring spins $j$ and $j+1$. We assume the standard energy normalisation whereby $\|h_j\| = O(1)$. The interaction $h_j$ may vary with position.

The objective of this Letter is to understand the distribution of eigenvalues for the operator $H$. To do this we’ll study the eigenvalue density function $\mu_H(x)$ for $H$ which is given by

$$\mu_H(x) = \frac{1}{2^n} \sum_{j=0}^{2^n-1} \delta(E_j - x),$$  

where $\delta(x)$ is the Dirac delta function and $E_j$ are the eigenvalues of $H$. The eigenvalue counting function $N_H(x)$ of $H$ is defined to be equal to the number of eigenvalues of $H$ which are less than or equal to $x$.

The eigenvalue density function $\mu_H(x)$ for an operator $H$ has a delta function spike at the position of each eigenvalue of $H$. Notice that we have normalised the eigenvalue density function $\mu_H(x)$ to have area 1, i.e. $\int_{-\infty}^{\infty} dx \mu_H(x) = 1$. We have done this principally so that we can compare the eigenvalue densities for operators on different Hilbert spaces. The eigenvalue counting function $N_H(x)$ can be expressed in terms of the eigenvalue density function $\mu_H(x)$ as $N_H(x) = 2^n \int_{-\infty}^{x} dw \mu_H(w)$.

We obtain the eigenvalue density function $\mu_H(x)$ for an operator $H$ via the following procedure. Write $H$ in its eigenbasis, $H = \sum_{j=0}^{2^n-1} E_j |E_j\rangle \langle E_j|$, and consider the propagator $U(t) = e^{itH} = \sum_{j=0}^{2^n-1} e^{iE_j t} |E_j\rangle \langle E_j|$. Taking the fourier transform of the scaled propagator $\frac{1}{2^n} U(t)$ yields

$$\frac{1}{2^n} \hat{U}(\omega) = \frac{1}{2^n} F[U(t)] = \frac{2\pi}{2^n} \sum_{j=0}^{2^n-1} \delta(E_j - \omega) |E_j\rangle \langle E_j|,$$

where the fourier transform pair $(\mathcal{F}[\cdot], \mathcal{F}^{-1}[\cdot])$ is defined to be $F(\omega) = \mathcal{F}[f(t)] = \int_{-\infty}^{\infty} dt f(t) e^{-i\omega t}$ and $f(t) = \mathcal{F}^{-1}[F(\omega)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt F(\omega) e^{i\omega t}$. If we take the trace of $\frac{1}{2^n} \hat{U}(\omega)$ we find $2\pi \mu_H(\omega) = \frac{1}{2^n} \text{tr}(\hat{U}(\omega)) = \frac{2\pi}{2^n} \sum_{j=0}^{2^n-1} \delta(E_j - \omega)$.

The calculations in the previous paragraph show that if we know $\text{tr}(U(t))$ for arbitrary times then we have enough information to extract $\mu_H(x)$. Now we show that if we only know an approximation $V(t)$ to $U(t)$ valid for some time $|t| \leq T$ then we can still extract an approximation $\mu_H(x)$ to $\mu_H(x)$ which can be systematically improved as $T$ is increased. The idea is to introduce a scalar-valued windowing function $\chi_T(t)$ which cuts off the propagators $U(t)$ and $V(t)$ outside $|t| \leq T$ so that $\chi_T(t)V(t) \sim \chi_T(t) U(t)$ for all $t$. One convenient choice for $\chi_T(t)$, which we use in the sequel, is the gaussian:

$$\chi_T(t) = e^{-\frac{t^2}{2\sigma^2}}.$$  

If we now study $\frac{1}{2^n} \chi_T(t) \text{tr}(U(t))$, rather than $\frac{1}{2^n} \text{tr}(U(t))$, then a fourier transform and an application of the convolution theorem yields

$$\frac{1}{2^n} \mathcal{F}[\chi_T(t) \text{tr}(U(t))] = \frac{2\pi}{2^n} \sum_{j=0}^{2^n-1} \hat{\chi}_T(E_j - \omega),$$  

where $\hat{\chi}_T(\omega)$ is the fourier transform of the windowing/characteristic function. It is straightforward to identify Eq. (3) as a convolution

$$\frac{1}{2^n} \mathcal{F}[\chi_T(t) \text{tr}(U(t))] = 2\pi (\hat{\chi}_T * \mu_H)(\omega).$$  

In this way we identify the fourier transform of $\frac{1}{2^n} \chi_T(t) \text{tr}(U(t))$ with a smearing of the eigenvalue density function $\mu_H(\omega)$ with a smearing function $\hat{\chi}_T(\omega)$. When $\chi_T(t)$ is chosen to be a gaussian, as in Eq. (3), it is clear that increasing the time window $T$ reduces the width of $\hat{\chi}_T(\omega)$. Thus, in the limit $T \to \infty$ we smoothly (but not uniformly!) recover the eigenvalue distribution function: $\mu_H(\omega) = \lim_{T \to \infty} (\hat{\chi}_T * \mu_H)(\omega)$.

It is immediate that if we now have only an approximation $V(t)$ to $U(t)$ which is good for $|t| \leq T$ then...
the fourier transform of \( g(t) = \frac{1}{T} \chi_T(t) \operatorname{tr} (V(t)) \) will be close to that of \( f(t) = \frac{1}{T} \chi_T(t) \operatorname{tr} (U(t)) \). One way to justify this is either to exploit the Parseval’s relation, i.e., that the fourier transform is a unitary operation on \( L_2 \), or to use the result that if \( \|f - g\|_1 \leq \epsilon \) then \( \| \hat{f} - \hat{g} \|_\infty \leq \epsilon \), where \( \| \cdot \|_1 \) and \( \| \cdot \|_\infty \) denote the \( L_1 \) and \( L_\infty \) norms, respectively.

We can also study the trace of the propagator in imaginary time: consider \( U(t + i\beta) = e^{-\beta H} e^{i\beta t} \). Taking the trace yields

\[
f(it + \beta) = \operatorname{tr} (U(t + i\beta)) = \sum_{j=0}^{2^n-1} e^{-\beta E_j} e^{iE_j t}.
\]

We obtain \( \mu_H \) from \( f(it + \beta) \) for a fixed \( \beta \) by computing the laplace transform inversion integral

\[
\mu_H(\omega) = \int_{\beta - i\infty}^{\beta + i\infty} ds f(s) e^{s\omega}.
\]

For a fixed \( \beta \) this can be done with an inverse fourier transform in \( t \): \( \mu_H(\omega) = e^{\beta \omega} 3^{-1} [f(it + \beta)] \). It is straightforward to see that if we only know an approximation \( V(t + i\beta) \leftrightarrow U(t + i\beta) \) valid for \( |t| \leq T \) then the fourier transform \( \tilde{g}(\omega) \) along \( t \) of the cutoff trace \( g(it + \beta) = \chi_T(t) \operatorname{tr} (V(t + i\beta)) \) provides a good approximation to \( e^{-\beta \omega} \tilde{X}_T \mu_H(\omega) \). Thus, after normalisation, \( e^{\beta \omega} \tilde{g}(\omega) \) provides a good representation for the smeared eigenvalue density function for \( \omega \sim E_0 \), where \( E_0 \) is the ground state energy. This representation becomes exponentially worse as \( \omega \) increases. By combining this representation with the one obtained from pure time evolution allows us to tradeoff the errors in the two representations.

The preceding discussion serves to establish the fact that a good approximation \( V(t) \leftrightarrow U(t) = e^{iHt} \) which is valid for complex times \( |t| \leq T \) provides sufficient information to resolve the eigenvalue distribution function on a lengthscale \( \delta \sim O(\frac{1}{T}) \). In the next part of this Letter we provide a numerical algorithm, closely related to the DMRG, which efficiently calculates a numerical representation for \( \tilde{X}_T \mu_H(\omega) \).

The crucial idea underlying our numerical method is that a good approximation \( V(t) \leftrightarrow U(t) \) for a local 1D quantum spin lattice system can be stored efficiently (i.e. with polynomial resources in \( n \)) on a classical computer for for \( |t| \leq T \), where \( T \sim O(\log(n)) \) (see also [12, 20]). See Fig. 1 for an illustration of the structure of the propagator \( e^{iHt} \) for an arbitrary local spin system. This result allows us to certify that our algorithm can correctly obtain an approximate representation for the smeared eigenvalue distribution function to within a constant lengthscale which can be arbitrarily large (but scaling at most logarithmically with \( n \)).

The way we actually store a representation for \( V(t) \) is as a matrix product operator (MPO) [18, 28]. What we mean by this is that we represent an operator \( W \in \mathcal{B}(\mathcal{H}) \) in the following fashion

\[
W = \sum_{j \in Q_n} A^{j_0} A^{j_1} \cdots A^{j_{n-1}} \sigma^{j_0} \otimes \cdots \otimes \sigma^{j_{n-1}},
\]

where \( Q_n = (\mathbb{Z}/4\mathbb{Z})^n \), and \( A^{j_0} \) and \( A^{j_{n-1}} \) are a collection of four \( C_0 \times 1 \) sized row vectors (respectively, four \( 1 \times D_{n-1} \) sized column vectors) and \( A^{j_k} \) are four \( C_k \times D_k \) sized matrices. Note that \( C_{k+1} = D_k \). The dimensions \( C_k \) and \( D_k \) are called the auxiliary dimensions for site \( k \). It is clear that if the sizes of the auxiliary dimensions are bounded by polynomials in \( n \), i.e. \( C_k \leq \text{poly}(n) \) and \( D_k \leq \text{poly}(n) \), then the operator \( W \) can be stored with polynomial resources in \( n \). Also note that all operators can be represented exactly as in Eq. (8) by taking the auxiliary dimensions to be large enough: \( C_k = D_k = 2^n \) suffices.

We obtain the MPO representation for \( V(t) \) via the following method. First we break \( H \) into two pieces \( A \) and \( B \) which contain the interaction terms on the even (respectively, odd) sites. Note that each term within \( A \) (respectively \( B \)) commutes with all the other terms within \( A \) (respectively, \( B \)). Then we exploit the Lie-Trotter expansion

\[
e^{iHt} = \lim_{m \to \infty} (e^{iA \frac{t}{m}} e^{iB \frac{t}{m}})^m,
\]

to write our expression for \( V(t) \), i.e., we pick some \( m \) and write \( V(t) = W^m \), where \( W = e^{iA \frac{t}{m}} e^{iB \frac{t}{m}} \). We next
\[ e^{i\hbar t} = \sum_{\alpha, \beta = 0}^{\delta} c[^3_{\alpha, \beta}] \sigma^j_{\alpha} \otimes \sigma^j_{\beta}, \]

By writing \( W \) in terms of the standard product operator basis we obtain the MPO representation
\[
W = \sum_{j \in Q_n} B^{(a)}_{\alpha} A^{j_1}_{\beta} \cdots A^{j_{n-1}}_{\mu} \sigma^{j_0} \otimes \sigma^{j_1} \otimes \cdots \otimes \sigma^{j_{n-1}},
\]

where \( B^{(a)}_{\alpha} = c^{[0]}_{\alpha, \alpha}, A^{j_0}_{\beta} = g^{j_0}_{\beta} c^{[k]}_{\beta} \) on even sites, \( A^{j_0}_{\beta} = g^{j_0}_{\beta} c^{[k]}_{\beta} \) on odd sites, and \( B^{(a)}_{\alpha} = \delta_{\alpha, 0} \).

Now we show that if two MPO’s \( J \) and \( K \) have maximum auxiliary dimensions \( D_J \) and \( D_K \) then \( JK \) is expressible as a MPO \( L \) with auxiliary dimension \( D_{JK} \leq D_J D_K \). Representing \( J = \sum_{j \in Q_n} A^{j_0}_{\alpha} A^{j_1}_{\beta} \cdots A^{j_{n-1}}_{\mu} \sigma^{j_0}_{0} \otimes \sigma^{j_1}_{1} \otimes \cdots \otimes \sigma^{j_{n-1}}_{n-1} \) and \( K = \sum_{j \in Q_n} B^{j_0}_{\alpha} B^{j_1}_{\beta} \cdots B^{j_{n-1}}_{\mu} \sigma^{j_0}_{0} \otimes \sigma^{j_1}_{1} \otimes \cdots \otimes \sigma^{j_{n-1}}_{n-1} \) and taking the product gives \( L = JK = \sum_{j \in Q_n} C^{j_0}_{\alpha} C^{j_1}_{\beta} \cdots C^{j_{n-1}}_{\mu} \sigma^{j_0}_{0} \otimes \sigma^{j_1}_{1} \otimes \cdots \otimes \sigma^{j_{n-1}}_{n-1} \), where
\[
C^{j_0}_{\alpha} = \sum_{j_1, \cdots, j_{n-1}} A^{j_0}_{\alpha} B^{j_1}_{\alpha} g^{j_1 \cdots j_{n-1}}_{k_1 \cdots k_{n-1}},
\]

We now apply this recipe to \( W^m = V(t) \). Obviously, after a couple of products, \( W^m \) potentially requires an exponentially large auxiliary dimension to represent it perfectly. It is here that we use a method similar to the DMRG truncation to reduce the size of this auxiliary dimension. We begin by representing \( W^l \) as an MPO perfectly for as large an \( l \) as possible. Then we minimise the Hilbert-Schmidt norm difference \( ||W^l - Y||_{HS} = \sqrt{\text{tr}((W^l - Y)^\dagger (W^l - Y))} \), where \( Y \) is a MPO with a smaller auxiliary dimension. This is a multiquadratic optimisation problem and can be solved numerically in polynomial resources in \( n \). (For a detailed description of this procedure see [2].) We then use the approximation \( Y \) to obtain an approximation \( YW \) to \( W^{l+1} \) and repeat this process for the desired number of iterations.

Given an approximation \( \tilde{V}(t) = \sum_{j \in Q_n} A^{j_0}(t) A^{j_1}(t) \cdots A^{j_{n-1}}(t) \sigma^{j_0} \otimes \sigma^{j_1} \otimes \cdots \otimes \sigma^{j_{n-1}} \) to \( U(t) \) as an MPO with bounded auxiliary dimension \( D \) it is straightforward to obtain the trace efficiently: \( \text{tr}(\sigma^n) = \delta_{n, 0} \) gives \( \text{tr}(\tilde{V}(t)) = A^{0}_0 A^{0}_0 \cdots A^{0}_{n-1} \).

This procedure provides us with a discrete representation \( g_k \sim \text{tr}(W^k), k = 0, 1, \ldots, m - 1 \), for an approximation to the trace \( f(t_k) \) of \( U(t_k) \). To obtain an approximate representation for \( \mu_H \) we apply a discrete fourier transform to \( g_k \sim \text{tr}(W^k) \) for some \( s \) chosen small enough to cutoff \( g_k \) completely by \( k_{\text{max}} \). A standard result of fourier analysis shows that this discrete representation will be a good representation for the smeared eigenvalue density function as long as we sample more rapidly than the Nyquist frequency \( \nu \). We can provide a bound for \( \nu \) by noting that the largest eigenvalue \( E_{\text{max}} \) of \( H \) satisfies \( E_{\text{max}} \leq ||H||_n \), which is \( O(n) \).

We have applied this numerical method to study the eigenvalue distribution function for a random antiferromagnetic Heisenberg model on 20 spins, see Fig. 2 and Fig. 4.

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[21] The eigenvalue density function should not be confused with the local density of states (LDOS) which is the distribution $p_j = |c_j|^2$ of coefficients of the state $A|E_0\rangle = \sum_{j=0}^{2^n-1} c_j |E_j\rangle$ in the energy eigenbasis, where $A$ is an arbitrary operator.
[22] By “good” we mean that, for some $\epsilon$, $\|U(t) - V(t)\| \leq \epsilon$, for $|t| \leq T$, where $\|\cdot\|$ denotes operator norm.