Efficiency of Free Energy Calculations of Spin Lattices by Spectral Quantum Algorithms

Cyrus P. Master,¹ Fumiko Yamaguchi,¹ and Yoshihisa Yamamoto¹,²
¹Quantum Entanglement Project, ICORP, JST, Stanford University, Stanford, CA 94305-4085
²NTT Basic Research Laboratories, 3-1 Morinosato-Wakamiya, Atsugi, Kanagawa 243-0198, Japan
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Quantum algorithms are well-suited to calculate estimates of the energy spectra for spin lattice systems. These algorithms are based on the efficient calculation of discrete Fourier components of the density of states. The efficiency of these algorithms in calculating the free energy per spin of general spin lattices to bounded error is examined. We find that the number of Fourier components required to bound the error in the free energy due to the broadening of the density of states scales polynomially with the number of spins in the lattice. However, the precision with which the Fourier components must be calculated is found to be an exponential function of the system size.

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I. INTRODUCTION

Spin lattice models are useful for the study of magnetic ordering in real materials. The dynamics of these models are specified by a Hamiltonian $\hat{H}$ involving spin operators for each of the $n$ lattice sites. Of particular interest is the behavior of thermodynamic functions – such as the magnetization, specific heat capacity, and magnetic susceptibility – across phase transitions. These functions are encapsulated in the dependence of the Helmholtz free energy – across phase transitions. These functions are specified by a Hamiltonian $\hat{H}$.

Calculation of the free energy for a general spin lattice model by conventional means is difficult. A naive approach is to enumerate the eigenenergies $\{E_m\}$ of $\hat{H}$, since

$$F = -n^{-1} k_B \theta \ln Z = -n^{-1} k_B \theta \ln \left( \sum_m e^{-\beta E_m} \right), \quad (1)$$

where $k_B \theta = \beta^{-1}$ is the thermal energy, and $Z$ is the partition function. However, as the number of eigenstates grows exponentially with the number of spins in the lattice, the time required to perform the calculation is prohibitively large. A variety of quantum Monte Carlo methods exist to calculate the free energy, including thermodynamic integration [12, 13], histogram methods [3, 4], and cumulant expansion [5, 6] techniques. However, the “sign problem” (see, for example, Ref. [7]) prevents application of these methods to arbitrary lattice Hamiltonians.

An alternate approach is available if one can efficiently generate an estimate of the density of states $\rho(E)$. As an approximation for the density of states $\rho(E)$ directly translates into an estimate $\tilde{F}$ for the free energy per spin.

Algorithms for quantum computers have been proposed to determine information about the spectra of Hermitian operators [8, 9, 10, 11, 12, 13]. We focus on algorithms [12, 13] that efficiently generate estimates of individual Fourier components $f_\ell$ of $\rho(E)$; they will be reviewed in detail in Section II. $N$ iterations of the algorithms yield $N$ Fourier components, from which an estimate of the density of states can be calculated.

An important issue that has not been addressed is the efficiency of these algorithms for calculating thermodynamic functions as a function of $n$. For the calculation to be deemed efficient, it must be shown that the computation time – and, thus, the number of Fourier components – required to calculate an estimate $\tilde{F}$ to bounded error scales polynomially with $n$. The bounded error criterion we adopt is

$$\text{Prob}\left( |\tilde{F} - F| < \gamma k_B \theta \right) > 1 - \epsilon, \quad (3)$$

where $\gamma$ and $\epsilon$ are small constants. Thus, the absolute error in the estimated free energy per spin must be smaller than a fraction of the thermal energy with probability arbitrarily close to one.

We examine the primary sources of error involved in the calculation of $F$ to determine the efficiency of the spectral algorithms. First, as only a finite number of Fourier components $f_\ell$ of the density of states are calculated, the estimated density of states is broadened relative to the actual function. This deterministic source of error (i.e., it is unchanged if the calculation is repeated) is reduced by increasing the number of components $N$, and thus the computation time. Second, there is an inherent stochastic source of error reflected in deviations in the estimated $f_\ell$ from the actual values. This error

*Electronic address: cpmaster@stanford.edu

References:
1. [12, 13]
2. [3, 4]
3. [5, 6]
could arise from imprecise implementation of logic gates or noise in the measurement process.

In this paper, we will show that if all of the $f_\ell$ are known exactly, the bound in Eq. (3) may be met by a number of Fourier components that scales polynomially with $n$. Thus, the error due to the broadening of the density of states does not prevent efficient estimation of the free energy per spin. However, the free energy becomes increasingly sensitive to random errors in each of the $f_\ell$ as the number of spins is increased. We will show that the precision of the output of the quantum algorithm must improve exponentially with $n$ in order to sustain the condition in Eq. (3). Thus, it is questionable as to whether spectral algorithms can be applied to the calculation of thermodynamic functions.

The paper is organized as follows: Section II reviews the quantum algorithms used to generate the components $f_\ell$, and discusses assumptions and expected properties of the spin Hamiltonian. Section III describes the calculation of $F$ from the Fourier components, and discusses the influence of sampling and window functions. In Section IV, we analyze the deterministic error due to broadening and determine the number of samples required to meet Eq. (3). In Section V, we analyze the impact of random deviations in the components $f_\ell$ on the estimated free energy.

II. QUANTUM ALGORITHMS

In this section, we review quantum algorithms for the calculation of the Fourier transform of the density of states. We describe a simple algorithm applicable only to Hamiltonians that are diagonal in the computational basis, and then discuss a more general algorithm applicable to ensemble quantum computers.

In regards to notation, we use the standard model for quantum computation, assuming our $p$ qubits to be two-level systems with logical states $|0\rangle_j$ and $|1\rangle_j$, $j \in \{0, 1, \ldots, p-1\}$, corresponding to eigenstates of the $\sigma_z(j)$ Pauli spin operator with eigenvalues $\pm 1$. The computational basis states for the quantum computer are denoted as $|x\rangle = |x_1\rangle_1 |x_2\rangle_2 \ldots |x_p\rangle_p$, where $\{x_j\}$ are the binary digits of the integer $x$. It is assumed that the quantum computer is capable of implementing a universal set of elementary single-qubit and two-qubit gates. The evolution time of these gates is an implementation-dependent constant, such that the overall computation time is reflected by the number of gates used in the algorithm.

We will restrict our discussion to lattices of spin-1/2 particles, as it is straightforward to map the eigenstates of $\sigma_z(j)$ in the spin system to the logical $|0\rangle_j$ and $|1\rangle_j$ states of qubit $j$ of the quantum computer. It should be noted that this restriction does not preclude the treatment of lattices of particles with spins larger than 1/2. Generalized Jordan-Wigner transformations exist to represent the dynamics of such lattices by a collection of spin-1/2 particles via intermediate fermionization.

Prior to the discussion of individual algorithms, we state three assumptions regarding the nature of the spin lattice Hamiltonian. First, we assume that the energy bandwidth $\Delta E$ – the energy difference between the ground state and the highest excited state – is bounded by a polynomial function of $n$. This assumption is likely to be valid for models of interest. As an example, consider a lattice of particles interacting by a nearest-neighbor XXZ interaction:

$$\hat{H} = \sum_{\langle i,j \rangle} J_z \left( \sigma_z^{(i)} \sigma_z^{(j)} + \sigma_y^{(i)} \sigma_y^{(j)} \right) + J_x \sigma_x^{(i)} \sigma_x^{(j)}.$$  (4)

The expectation value of the summand in Eq. (4) must lie between $-(2|J_z| + |J_x|)$ and $(2|J_z| + |J_x|)$. The number of terms in the summation is equal to $n/2$ times the coordination number for the lattice, implying that the energy bandwidth is bounded by a function linear in $n$.

In general, for any Hamiltonian involving only pairwise interactions between spins (of $n$-independent interaction energy), it is evident that the energy bandwidth is $O(n^2)$.

Second, we assume that the time-evolution operator $\hat{U}(t) \equiv \exp(-i\hat{H}t)$ can be implemented as a sequence of elementary single-qubit and two-qubit gates, where the number of gates is a polynomial function of $n$. In cases where the Hamiltonian consists of commuting pair-wise interactions (e.g., the Ising model), this decomposition is trivial. Otherwise, one may use a Trotter-Suzuki expansion of non-commuting terms to implement $\hat{U}(t)$ to arbitrarily small error.

Finally, we assume that the energy scale is shifted such that the eigenenergies fall between $E = 0$ and $E = \Delta E$. This last assumption is made for mathematical convenience, and does not affect the results of our analysis.

The following algorithms are based on the fact that the Fourier transform of the density of states $\rho(E)$ is equal to the trace of the time evolution operator:

$$f(t) \equiv \int_{-\infty}^{\infty} \rho(E) e^{-iEt} dE = \text{Tr} \left( e^{-i\hat{H}t} \right).$$  (5)

As $|f(t)| \leq 2^n$, it is convenient to define a function

$$g(t) \equiv \frac{1}{2^n} f(t) = \frac{1}{2^n} \text{Tr} \left( e^{-i\hat{H}t} \right),$$  (6)

such that $|g(t)| \leq 1$. The algorithms described in this section calculate samples of $g(t)$ at discrete times $t_\ell$.

Before discussing the general case, it is illuminating to examine a simple algorithm restricted to spin lattices for which $\hat{H}$ is diagonal in the computational basis. As an example, one might consider a nearest-neighbor Ising model in a longitudinal magnetic field:

$$\hat{H} = J_z \sum_{\langle i,j \rangle} (1 - \sigma_z^{(i)} \sigma_z^{(j)}) + \hbar \sum_j (1 - \sigma_x^{(j)}).$$  (7)
The gates shown in Fig. 1 for an $n$-qubit computer can be used to calculate the magnitude of $g(t_{\ell}) \equiv g_{\ell}$. The quantum computer is initialized to the $|0\rangle$ state. The gate $W$ corresponds to a sequence of Walsh-Hadamard gates $W_j$ for each qubit $j$:

$$\begin{align*}
W_j : & \left\{ 
\begin{array}{c}
|0\rangle_j \rightarrow \frac{1}{\sqrt{2}} \left( |0\rangle_j + |1\rangle_j \right), \\
|1\rangle_j \rightarrow \frac{1}{\sqrt{2}} \left( |0\rangle_j - |1\rangle_j \right) \end{array} \right. ,
\end{align*}$$

The gate $U(t_{\ell})$ corresponds to the time evolution operator.

As a final step, a projective measurement is performed in the computational basis. It is straightforward to show that the probability of observing all qubits in the logical $|0\rangle$ state is equal to $|g_{\ell}|^2$:

$$
|0\rangle \xrightarrow{W} \frac{1}{\sqrt{2^n}} \sum_{m=0}^{2^n-1} |m\rangle \xrightarrow{U(t_{\ell})} \frac{1}{\sqrt{2^n}} \sum_{m=0}^{2^n-1} e^{-iE_m t_{\ell}} |m\rangle \xrightarrow{W} g_{\ell} |0\rangle + \text{orthogonal components}.
$$

By assumption, the computational basis states $|m\rangle$ are eigenstates of the Hamiltonian, and the time-evolution operator appends a phase proportional to the eigenvalue $E_m$ to each term. An unbiased estimator for $|g_{\ell}|$ can be derived by performing $R$ repetitions of the algorithm $R$, and counting the number of times all qubits are found in the logical $|0\rangle$ state.

The magnitude of $g_{\ell}$ is insufficient to reconstruct the density of states. By adding an ancilla qubit $a$, as shown in Fig. 2, one may extract estimates of both the real and imaginary parts of $g_{\ell}$. The $X$ gate and $R$ iterations with the $Y$ gate, one can derive estimators $\hat{p}$ for the probabilities. Unbiased estimates of the real and imaginary parts of $g_{\ell}$ are

$$\begin{align*}
\text{Re} (\hat{g}_{\ell}) &= (\hat{p}_{Y_0} - \hat{p}_{Y_1}), \\
\text{Im} (\hat{g}_{\ell}) &= (\hat{p}_{X_1} - \hat{p}_{X_0}).
\end{align*}$$

We use the tilde to distinguish estimates of the Fourier components obtained from the quantum algorithm from the exact values.

The algorithm described above depends on our ability to construct an equally-weighted coherent superposition of eigenstates of $\hat{H}$; hence, the restriction to Hamiltonians that are diagonal in the computational basis. It can be generalized \[14\] by considering an algorithm involving an ensemble of quantum computers, such that the ancilla qubit is still initialized to the $|0\rangle_a$ state, but the remaining $n$ qubits are in a completely random mixed state. The initial density matrix for the system is

$$\hat{\rho}_i = \frac{1}{2^{n+1}} \left( \hat{I}^{(a)} + \hat{\sigma}^{(a)}_z \right) \hat{I}^{(q_1)} \hat{I}^{(q_2)} \cdots \hat{I}^{(q_n)},$$

where $\hat{I}^{(\ell)}$ is the identity operator for qubit $\ell$. The operator $\hat{I}^{(q_1)} \hat{I}^{(q_2)} \cdots \hat{I}^{(q_n)}$ is equal to the resolution of the identity $\sum_\ell |\psi_\ell\rangle \langle \psi_\ell|$ where $\{|\psi_\ell\rangle\}$ is an orthogonal set of states in the subspace spanned by qubits $q_1$ through $q_n$. One could use as $\{|\psi_\ell\rangle\}$ the eigenstates of the Hamiltonian $\hat{H}$. We do not need to explicitly solve for the eigenstates of $\hat{H}$; the initial density matrix can be thought of as an incoherent mixture of eigenstates for any Hamiltonian $\hat{H}$.

If the coherent superposition created by the Walsh-Hadamard gates is replaced by such an incoherent mixture, then an algorithm nearly identical to the one shown above works for any choice of $\hat{H}$, as shown in Fig. 3. The final measurement is the expected value of $\hat{\sigma}^{(a)}_z$ averaged over the ensemble.

If the $X$ gate is used for the ancilla qubit, the expected value of $\hat{\sigma}^{(a)}_z$ is

$$\langle \hat{\sigma}^{(a)}_z \rangle = \text{Im} (g_{\ell}),$$

\[ \text{FIG. 1: Logic diagram of an elementary algorithm to estimate } |g_{\ell}|. \]

\[ \text{FIG. 2: Logic diagram of an algorithm to estimate the real and imaginary parts of } g_{\ell} \text{ for diagonal } \hat{H}. \]
Fourier transform in the context of windowing and sampling of the exact function of \( \rho(E) \), the reconstructed estimate \( \tilde{\rho}(E) \), translates into error in \( \tilde{\rho}(E) \) relative to the exact function \( \rho(E) \). This distortion translates into error in the estimate of the free energy. The density of states, \( \rho(E) \), are weighted by a windowing function \( b_\ell(t) \). If \( n \) is small compared to the thermal energy, \( \rho(E) \), the initial density matrix of the system is well-approximated by the identity operator. The single elementary gates. Second, initial state preparation lends itself to ensemble quantum computation proposals involving spin resonance, where the Zeeman splitting between qubit spin states is small compared to the thermal energy.

In equilibrium, the initial density matrix of the system is small compared to the thermal energy.

As iterations of the quantum algorithm yield discrete samples of \( f(t) \), the reconstructed estimate \( \tilde{\rho}(E) \) is distorted relative to the exact function \( \rho(E) \). This distortion translates into error in \( \tilde{F} \). It is convenient to view this error in the context of windowing and sampling of the exact Fourier transform \( f(t) \) of the density of states. Truncation of \( f(t) \) to a window of width \( T_0 \) centered about \( t = 0 \) (i.e., multiplication of \( f(t) \) by a windowing function \( b_\ell(t) \)) that is constant for \( |t| \leq T_0/2 \) and zero elsewhere) leads to a convolution of the density of states by a broadening function \( b_\ell(t) \equiv \alpha_1 \sin(\frac{\pi t}{T_0}) = \alpha_1 \frac{\sin(\frac{\pi t}{T_0})}{T_0} \), where the energy resolution \( \Delta E \) is given by

\[
\Delta E = \frac{2\pi}{T_0}.
\]

The window is scaled such that the broadening function is normalized to unit area; i.e., \( \alpha_1 = 1/\Delta E \). Increasing the window size \( T_0 \) reduces the width of the broadening function, and thus the error in the estimate of \( \tilde{F} \).

The effect of sampling on the estimated density of states can be determined by multiplying \( f(t)b_\ell(t) \) by an impulse train \( s(t) \) of spacing \( \Delta t \):

\[
s(t) = \Delta t \sum_{\ell=-\infty}^{\infty} \delta(t - \ell \Delta t).
\]

Sampling leads to periodic replication of the broadened \( \rho(E) \). The resultant density of states is given by the Fourier transform of \( f(t)b_\ell(t)s(t) \):

\[
\rho'(E) \equiv \rho(E) * b_\ell(E) * \sum_{k=-\infty}^{\infty} \delta \left( E + \frac{2\pi k}{\Delta t} \right). \tag{19}
\]

To avoid aliasing in the estimated density of states, the Nyquist sampling condition requires that

\[
\Delta t \leq \frac{2\pi}{\Delta E}. \tag{20}
\]

The spacing between samples of \( f(t) \) is determined solely by the estimate of the energy bandwidth, \( \Delta E \). We assume that sampling is performed at the Nyquist rate, and the equality holds in Eq. (20).

As the number of samples is equal to the ratio of the windowing function width \( T_0 \) to the sampling time, one could determine the minimum value of \( T_0 \) required to satisfy Eq. (20) as a function of \( n \). However, the rectangular windowing function leads to poor results. The envelope of the associated broadening function \( b_1(E) \) falls off weakly as \( 1/E \); the oscillating side lobes are amplified at low energies by the Boltzmann factor in the calculation of the free energy. The window width required to mitigate the resultant error scales poorly with \( n \). In contrast to using wider rectangular windows, one may adopt more elaborate window shapes whose corresponding broadening functions exhibit envelopes that are more

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**FIG. 3:** Logic diagram of an ensemble algorithm to determine \( g_\ell \) for arbitrary \( \mathcal{H} \).

**FIG. 4:** Block diagram of the calculation of \( \tilde{F} \).
sharply peaked. We consider the functions \( b_\theta(t) \) formed by the successive convolution of \( \Theta \) rectangular windows, each of width \( T_0 \). \( \Theta \) is referred to as the order of the windowing function. For \( \Theta = 2 \), the window is triangular and of width \( 2T_0 \). With increasing order, the window approaches a Gaussian shape, and is of width \( \Theta T_0 \). The resulting broadening function is then

\[
b_\theta(E) = \alpha_\theta \left[ \text{sinc} \left( \frac{\pi E}{\Delta e} \right) \right]^\Theta, \tag{21}\]

which exhibits a \( 1/E^\Theta \) envelope. The value of \( \alpha_\theta \) is determined, as the area under \( b_\theta(E) \) is one. In practice, a given window shape is constructed by obtaining samples \( f_t \) within the window width \( \Theta T_0 \) centered at \( t = 0 \), and weighting each sample by \( b_{\theta,t} = b_\theta(t) \).

As the envelope of the side lobes of \( b_\theta(E) \) falls off exponentially with \( \Theta \), windowing functions of large order significantly reduce the error in the calculated free energy. However, the tradeoff is a wider window, leading to more Fourier components, and thus more iterations of the quantum algorithm:

\[
N = \frac{\Theta T_0}{\Delta t}. \tag{22}\]

Therefore, the question of how \( N \) scales with the number of spins, \( n \), translates into the determination of the minimum values of \( \Theta \) and \( T_0 \) required to satisfy Eq. (3).

An estimate \( \tilde{Z} \) for the partition function can be calculated directly from the estimated Fourier components without intermediate calculation of the density of states. We denote quantities obtained from the quantum algorithm with a tilde, in contrast to their exact values. First, note that the Fourier transform of \( f(t) \) is bounded by Eq. (18) to give an estimate of the broadened, periodically replicated density of states \( \tilde{\rho}'(E) \) in terms of the components \( f_t \):

\[
\tilde{\rho}'(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) \left( \Delta t \sum_{\ell=-\infty}^{\infty} \delta(t - \ell \Delta t) \right) e^{iEt} dt = \frac{\Delta t}{2\pi} \sum_{\ell} f_{\theta,\ell} e^{iEt}, \tag{23}\]

where we have defined \( t_\ell \equiv \ell \Delta t \), and the sum is performed over all \( t_\ell \) within the window described by \( b_{\theta,\ell} \).

Integrating Eq. (23) over the energy bandwidth and using Eqs. (6) and (21), one finds

\[
\tilde{Z} = \int_0^{\Delta E} \rho'(E)e^{-\beta E} dE = \frac{2^\Theta \Delta t}{2\pi \beta} \left( 1 - e^{-\beta \Delta E} \right) \left\{ b_{\theta,0} + 2 \sum_{\ell>0}^{N/2} b_{\theta,\ell} \left[ \frac{1}{1 + (t_\ell/\beta)^2} \text{Re}(\tilde{g}_\ell) - \frac{t_\ell/\beta}{1 + (t_\ell/\beta)^2} \text{Im}(\tilde{g}_\ell) \right] \right\}. \tag{24}\]

Note that an estimate \( \tilde{F} \) of the free energy may be obtained from the logarithm of Eq. (24).

In addition to describing how an estimate of the free energy per spin is calculated from the Fourier components, Eq. (24) will serve as a starting point to determine the probabilistic error in \( \tilde{F} \) due to imprecise values of \( \tilde{g}_\ell \).

**IV. ERROR ANALYSIS: BROADENING**

In this section, we determine an upper bound on the number of samples \( N \) of \( g(t) \) required to calculate the free energy to the tolerance prescribed by Eq. (6). At this point, we consider the individual samples of \( g_\ell \) to be known exactly, and only consider the error in \( \tilde{F} \) due to the finite number of Fourier components – i.e., due to broadening of the density of states. With this restriction, we can show that \( N \) is a polynomial function of the number of spins \( n \).

As it is more convenient to work with the partition function than the free energy, we use a more stringent bound based upon the relative error in the calculated partition function \( \tilde{Z} \). As

\[
|\tilde{F} - F| < \gamma k_B \theta \iff e^{-\gamma n} - 1 < \frac{\tilde{Z} - Z}{Z} < e^{\gamma n} - 1, \tag{25}\]

it is sufficient to demand that

\[
\text{Prob} \left( r \equiv \left| \frac{\tilde{Z} - Z}{Z} \right| < \xi \right) > 1 - \epsilon, \tag{26}\]

where \( \xi \equiv 1 - \exp(-\gamma n) \). Note that \( \xi < 1 \), and in the limit \( \gamma n \ll 1, \xi \to \gamma n \).

By Eqs. (17), (20) and (22), if the Nyquist sampling condition is satisfied, then

\[
N = \frac{\Theta \Delta E}{\Delta e}. \tag{27}\]

It has been asserted that \( \Delta E \) is a polynomial function of \( n \). In the remainder of this section, we examine the dependence of \( \Theta \) and \( \Delta e \) on \( n \) such that Eq. (26) is satisfied. We require a pair of intermediate results:

**Lemma 1** If \( b_\theta(E) \) (as defined in Eq. (21)) is subject
to the normalization condition \( 1 = \int_{-\infty}^{\infty} b_\Theta(E)dE \), then
\[
\alpha_\Theta < \frac{c_\pi}{\Delta e} \sqrt{\frac{\Theta}{6\pi}}, \tag{28}
\]
where \( c \approx 2.0367 \).

\[\text{Lemma 2.}\]

\[ A_{\text{side}} \equiv 1 - \int_{-\Delta e}^{\Delta e} b_\Theta(E)dE < \frac{c}{\pi^33} \sqrt{\frac{\Theta}{6\pi}}, \tag{29}\]

where \( \Theta \) is an even integer.

Lemma 1 places an upper bound on \( \alpha_\Theta \) such that \( b_\Theta(E) \) is normalized. Lemma 2 states an upper bound on the area of \( b_\Theta(E) \) that is outside of the interval \([-\Delta e, \Delta e]\) (i.e., outside the main lobe of the broadening function) that decreases exponentially with \( \Theta \). Both are proved in the Appendix. Note that the proof of Lemma 2 applies to the case where \( \Theta \) is even.

One can relate the relative error \( r \) in the calculated partition function to the parameters \( \Theta \) and \( \Delta e \) via Lemma 2. As the exact density of states \( \rho(E) \) may be expressed as a sum of delta functions for each eigenenergy \( E_m \), Eqs. (19)-(20) at the Nyquist condition yield

\[
\tilde{Z} = \int_{0}^{\Delta E} \tilde{\rho}(E)e^{-\beta E}dE = \sum_m \sum_{k=-\infty}^{\infty} \int_{0}^{\Delta E} b_\Theta(E-E_m+k\Delta E)e^{-\beta E}dE = \sum_m \left[ \sum_{k=-\infty}^{\infty} \int_{k\Delta E}^{(k+1)\Delta E} b_\Theta(E-E_m)e^{-\beta(E-k\Delta E)}dE \right] = \sum_m \tilde{Z}_m. \tag{30}\]

The change of variables allows one to view \( \tilde{Z}_m \) as an integral of the broadening function, centered at \( E_m \), and weighted by periodically-replicated segments of an exponential function. \( \tilde{Z} \) is found by summing over all eigenenergies.

The maximum relative error \( r \) in the partition function is bounded by the largest contribution \( r_m = \max_m \left| \frac{\tilde{Z}_m - Z_m}{Z_m} \right| \) from any single eigenenergy, where \( Z_m = e^{-\beta E_m} \). Define \( \gamma_m = \tilde{Z}_m/Z_m \). Then,

\[
\left| \frac{\tilde{Z} - Z}{Z} \right| = \left| \sum_m \left( \frac{\tilde{Z}_m - Z_m}{Z_m} \right) \right| = \frac{\left| \sum_m (\gamma_m - 1)Z_m \right|}{\sum_m Z_m} \leq \max_m |\gamma_m - 1| = \max_m \left| \frac{\tilde{Z}_m - Z_m}{Z_m} \right| = r_m. \tag{31}\]

This argument shows that one may consider a simplified system with just one eigenstate at an energy \( E_m \) somewhere in the energy bandwidth. An upper bound on the error \( r \) for this simplified system for any \( E_m \) suffices to bounded the error for an arbitrary energy spectrum over the same bandwidth.

Lower and upper bounds on \( \tilde{Z}_m \) (\( \tilde{Z}_{m,\text{min}} \) and \( \tilde{Z}_{m,\text{max}} \), respectively) are now derived to bound \( r_m \), since

\[
r_m < \max \left( \left| \frac{\tilde{Z}_{m,\text{min}} - Z_m}{Z_m} \right|, \left| \frac{\tilde{Z}_{m,\text{max}} - Z_m}{Z_m} \right| \right). \tag{32}\]

In the main lobe, the minimum value of the Boltzmann factor is \( e^{-\beta(E_m+\Delta e)} \). Outside of the main lobe, the minimum value is \( e^{-\beta \Delta E} \).

Thus,

\[
\tilde{Z}_m = \sum_{k=-\infty}^{\infty} \int_{k\Delta E}^{(k+1)\Delta E} b_\Theta(E-E_m)e^{-\beta(E-k\Delta E)}dE \geq (1 - A_{\text{side}})e^{-\beta(E_m+\Delta e)} + A_{\text{side}}e^{-\beta \Delta E} \equiv \tilde{Z}_{m,\text{min}}. \tag{33}\]

Similarly, as the maximum value of the Boltzmann factor is \( e^{-\beta(E_m-\Delta e)} \) inside the main lobe and one outside,

\[
\tilde{Z}_m \leq (1 - A_{\text{side}})e^{-\beta(E_m-\Delta e)} + A_{\text{side}} \equiv \tilde{Z}_{m,\text{max}}. \tag{34}\]

Substituting Eqs. (33) and (34) into Eq. (32), we see that

\[
r_m < \max \{ 1 - (1 - A_{\text{side}})e^{-\beta \Delta e} - A_{\text{side}}e^{-\beta(\Delta E-E_m)}, (1 - A_{\text{side}})e^{\beta \Delta e} + A_{\text{side}}e^{\beta E_m} - 1 \}. \tag{35}\]

It is difficult to invert Eq. (35) explicitly to find optimal conditions on \( A_{\text{side}}(\Theta) \) and \( \Delta e \) that ensure that \( r_m < \xi \). However, one can show that the following conditions are sufficient:

\[
\beta \Delta e = \ln(1 + \xi/2), \tag{36}\]

\[A_{\text{side}} < \frac{\xi}{2} e^{-\beta \Delta E}. \tag{37}\]

As proof of their sufficiency, note that

\[
1 - (1 - A_{\text{side}})e^{-\beta \Delta e} - A_{\text{side}}e^{-\beta(\Delta E-E_m)} < \frac{\xi}{2} + \frac{\xi}{2} e^{-\beta \Delta e} \left( 1 - \frac{\xi}{2} \right) < \xi; \tag{38}\]

and,

\[
(1 - A_{\text{side}})e^{\beta \Delta e} + A_{\text{side}}e^{\beta E_m} - 1 < \frac{\xi}{2} + \frac{\xi}{2} e^{\beta(\Delta E-E_m)} < \xi. \tag{39}\]

Therefore, the conditions in Eqs. (36) and (37) guarantee that \( r_m < \xi \), as desired.

Using Lemma 2, one can manipulate Eqs. (36) and (37) to show that \( N \) scales polynomially with \( n \),

\[
\Delta e = \frac{\ln(1 + \xi/2)}{\beta}, \tag{40}\]

\[
\Theta - \frac{\ln \Theta}{2n} > \frac{\beta \Delta E}{n} + \frac{\ln(1/\xi)}{n} + \kappa, \tag{41}\]
where \( \kappa = 5/2 + \frac{\ln(2\nu/\sqrt{5})}{\ln \pi} \approx 2.9443 \). As \( \ln \Theta < \Theta \), a sufficient condition to satisfy Eq. (11) is

\[
\Theta/2 = [\mu \beta \Delta E + \mu \ln(1/\xi) + \kappa'],
\]

where \( \mu = 1/(2 \ln \pi - 1) \) and \( \kappa' = \mu \kappa \ln \pi \).

In summary, the error bound on the partition function is satisfied if the energy resolution scales linearly with temperature, and if \( \Theta \) scales linearly with \( \beta \Delta E \).

As a final step, we substitute the conditions in Eqs. (10) and (12) into Eq. (27), disregarding the weak logarithmic dependence of \( \Theta \) and \( \Delta E \) on \( n \):

\[
N = \frac{\Theta \Delta E}{\Delta \epsilon} \propto \frac{(\beta \Delta E)(\Delta E)}{1/\beta} = \beta^2(\Delta E)^2 \propto \text{poly}(n),
\]

by the assertion that the energy bandwidth is a polynomial function of the number of spins in our system. This result shows that in the absence of error in the calculated Fourier components of the density of states, the free energy per spin can be determined efficiently to bounded error.

V. ERROR ANALYSIS: FOURIER COMPONENTS

We now consider random errors in the individual values of \( \hat{g}_i \), which may arise from imprecise implementation of logic gates, or noise in the measurement process. Treating \( \text{Re}(\hat{g}_i) \) and \( \text{Im}(\hat{g}_i) \) as random variables, these fluctuations are modelled by their variances. We assume that the variances \( \sigma_g^2 \) are independent of \( i \). In this section, the dependence of the maximum allowable value of \( \sigma_g^2 \) on \( n \) such that Eq. (3) is maintained is derived.

As the estimate for the partition function \( Z \) is a linear combination of the independent random variables \( \text{Re}(\hat{g}_i) \) and \( \text{Im}(\hat{g}_i) \), the variance of \( Z \) can be calculated from Eq. (29):

\[
\sigma_Z^2 = 4^{n+1} \left( \frac{\Delta t}{2\pi \beta} \right)^2 (1 - e^{-\beta \Delta E})^2 \sum_{\ell=0}^{N/2} b^2_{\ell} \frac{\ell!}{(\ell + (t/\beta))^2}.
\]

(44)

If we assume that \( Z \) is Gaussian-distributed \( \mathcal{N} \), then the probability of \( Z \) deviating from its exact value \( Z \) can be related to the variance. Thus, the sum in Eq. (44) is evaluated by making two simplifications. First, we model the windowing function \( b_\Theta(t) \) as a Gaussian. Recall that \( b_\Theta(t) \) is constructed by the convolution of \( \Theta \) rectangular windows of width \( T_\Theta \). In the limit of large \( \Theta \), \( b_\Theta(t) \) may be approximated \( \mathcal{N} \) by

\[
b_\Theta(t) \approx e^{-t^2/2\nu^2},
\]

(45)

where \( \nu^2 = \Theta T_\Theta^2/12 \). Although this approximation over-estimates \( b_\Theta(t) \) away from \( t = 0 \), the fractional error in Eq. (44) incurred by the approximation is less than \( 5 \times 10^{-3} \) for \( \Theta > 40 \). Second, it is assumed that \( \beta/\Delta t = \beta \Delta E/2\pi \gg 1 \). The energy bandwidth is thus much larger than the thermal energy. This condition assures that the sum can be well-approximated by the integral

\[
\sigma_Z^2 \approx 4^{n+1} \left( \frac{\Delta t}{2\pi \beta} \right)^2 \int_0^{\infty} \frac{e^{-t^2/\nu^2}}{1 + t^2/\beta^2} dt
\]

\[
= 4^{n} \frac{\sigma_g^2}{\beta \Delta E} e^{\beta^2/\nu^2} [1 - \text{erf}(\beta/\nu)].
\]

(46)

Eq. (46) indicates that the standard deviation of \( Z \) scales exponentially with \( n \); i.e., as \( 2^n \). Note that the exact partition function \( Z \) will typically be a more slowly increasing function of \( n \). If the energy eigenvalues are limited to the domain \([0, \Delta E]\), then \( 2^n \) is an upper bound for the value of the partition function (achieved at infinite temperature, or if all eigenstates are degenerate with zero energy). Consider two simple examples. For the case of \( n \) non-interacting spins in a magnetic field with Zeeman energy \( h \), \( Z = (1 + e^{-\beta h})^n < 2^n \); for a linear chain Ising model in zero magnetic field, described by Eq. (6), \( Z = (1 - e^{-2\beta J})^n \) for periodic boundary conditions. Thus, if the distribution function for \( Z \) is Gaussian, one expects that the standard deviation increases exponentially faster than the mean \( Z \).

The above result may be used to derive a condition on \( \sigma_g^2 \) such that the error bound on the free energy per spin is fulfilled. By Eq. (3), the condition \( |F - 
\]

(47)

Assuming a Gaussian distribution for \( Z \) centered about \( Z \),

\[
\epsilon = 1 - \text{Prob}(Z < Z - \epsilon Z) \epsilon < \epsilon Z < \epsilon Z
\]

(48)

This result can be simplified if we consider the limit \( \gamma n \ll 1 \), such that \( e^{\pm \gamma n} \approx 1 \pm \gamma n \); i.e., for small desired absolute error in the free energy relative to the number of spins:

\[
\epsilon = \text{erf} \left( \frac{Z \gamma n}{\sqrt{2}\sigma_g} \right) \approx \text{erf} \left( \sqrt{\frac{\beta \Delta E}{2}} Z \gamma n \right).
\]

(49)

The argument of the \( \text{erf}() \) function must be order unity or larger for \( \epsilon < 0.1 \), so

\[
\sigma_g^2 = O \left( \frac{Z^{2} \text{poly}(n)}{4^n} \right).
\]

(50)

By the above argument, the variance in the measured Fourier components must decrease exponentially with \( n \).

The condition on \( \sigma_g^2 \) is likely to translate into an exponentially scaling computation time for the overall calculation. For example, consider as a quantum computer an
ensemble of spin-1/2 nuclei, where readout is performed by measuring the voltage induced in a pickup coil by free induction. A source of error in the measured Fourier components is the Johnson-Nyquist voltage noise due to the resistance of the coil [20]. The variance in the observed voltage – and thus in the estimates for $\text{Re}(g_f)$ and $\text{Im}(g_f)$ – is inversely proportional to the measurement time. Thus, Eq. (14) implies that an exponentially long measurement time is required to satisfy the condition in Eq. (3).

VI. CONCLUSION

We examined the applicability of spectral quantum algorithms for the calculation of the free energy of spin lattice models. Provided that the time-evolution operator for the system is decomposable into an efficient number of elementary gates, an ensemble quantum algorithm exists to generate estimates of the density of states by calculating individual Fourier components of $\rho(E)$. We analyzed the efficiency of this algorithm in calculating the free energy per spin of the system to bounded absolute error.

The error in the calculated free energy arises from the calculation of only a discrete number of Fourier components $f_\ell$, as well as from deviations in the measured values of $f_\ell$ due to statistical errors. The first source of error, attributable to broadening in the estimated density of states, was shown to lead to bounded error with a number of Fourier components that is polynomial in $n$. Thus, if the components $f_\ell$ are known exactly, the spectral algorithm is an efficient means to calculate the free energy per spin. However, the effect of random deviations in the calculated values of $f_\ell$ grows with increasing $n$. As the size of the system increases, the maximum tolerable variance in measured Fourier components decreases as $Z^2/4^n$ for large $n$ and small absolute error. As an upper bound for the partition function is $2^n$, the spectral algorithms are not an efficient method to determine $F$ in the presence of statistical errors in $f_\ell$.

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APPENDIX A: PROOFS OF LEMMERS 1 AND 2

Proof of Lemma 1: A lower bound is first derived for

\[ I \equiv \int_{-\infty}^{\infty} [\text{sinc}(x)]^\Theta \, dx = \int_{-\infty}^{\infty} e^{\Theta \ln[\text{sinc}(x)]} \, dx. \quad (A1) \]

We exclude infinitesimal regions around \( x = m\pi \) (\( m \in \mathbb{Z} \)) from the integral to avoid divergence of the logarithm; as \( \text{sinc}(x) \) approaches a finite value in these regions, the contribution of these regions to the integral can be made arbitrarily small.

Using a series expansion for \( \ln[\text{sinc}(x)] \) [2],

\[
\ln[\text{sinc}(x)] = -\frac{x^2}{6} - \sum_{k=2}^{\infty} \frac{x^{2k}}{k^2 \pi^{2k}} \left( \sum_{n=1}^{\infty} \frac{1}{n^{2k}} \right)
\]

\[
> -\frac{x^2}{6} - \left( \frac{x}{6} \right)^2 \sum_{k=2}^{\infty} \frac{x^{2k}}{k^2 \pi^{2k}}. \quad (A2)
\]

Thus,

\[
I > \int_{-\infty}^{\infty} e^{-\Theta x^2/6} e^{-\frac{x^2}{6} \sum_{k=2}^{\infty} \frac{x^{2k}}{k^2 \pi^{2k}}} \, dx. \quad (A3)
\]

The integrand is positive over the entire domain of \( x \), and both exponential factors monotonically decrease with \( |x| \). Thus, one may place a lower bound on \( I \) by reducing the limits of integration to any finite interval, such as \( |x| < \sqrt{6/\Theta} \).

Thus,

\[
I > e^{-\frac{\alpha^2 x^2}{6} + \sum_{k=2}^{\infty} \Theta \frac{n \alpha^2}{k^2 \pi^{2k}}} \int_{-\sqrt{6/\Theta}}^{\sqrt{6/\Theta}} e^{-\Theta x^2/6} \, dx. \quad (A4)
\]

The integral is \( \sqrt{6\pi/\Theta} \, \text{erf}(1) \). The summation can be performed explicitly to yield

\[
I > e^{1+\pi^2 \Theta /6} \Theta \ln(1-6/\pi^2 \Theta)/6 \sqrt{6\pi/\Theta} \, \text{erf}(1)
\]

\[
= e \left( 1 - \frac{6}{\Theta \pi^2} \right) \Theta \pi^2/6 \sqrt{6\pi/\Theta} \, \text{erf}(1)
\]

\[
> e \left( 1 - \frac{6}{\Theta \pi^2} \right) \pi^2/6 \sqrt{6\pi/\Theta} \, \text{erf}(1). \quad (A5)
\]

where we make use of the fact that \((1-1/x)^x\) is a monotonically increasing function for \( x > 1 \).

This lower bound for \( I \) is used to establish an upper bound for \( \alpha_\Theta \).

\[
\alpha_\Theta = \frac{1}{\int_{-\infty}^{\infty} [\text{sinc}(\frac{x}{\Theta})]^\Theta \, dE}
\]

\[
= \frac{\Delta e \, I}{\int_{-\Delta e}^{\Delta e} \sqrt{\Theta}} \quad (c \sqrt{\Theta}, \quad (A6)
\]

where \( c \) is defined as

\[
c \equiv \frac{1}{e} \left( \frac{1}{1 - 6/\pi^2} \right)^{7/6} \frac{1}{\text{erf}(1)} \approx 2.0367. \quad (A7)
\]

Proof of Lemma 2: For \( \Theta \) even, \( b_\Theta(E) \) is a non-negative function with unit area. If one treats \( b_\Theta(E) \) as a probability density function, one can use the Markov inequality to bound the area outside of the main lobe.

Consider a random variable \( Y \) with support \( y \geq 0 \); i.e., \( Y \) only takes non-negative values. Markov’s inequality bounds the probability of deviations from the mean:

\[
Pr \left( Y \geq \delta \right) \leq \frac{E(Y)}{\delta}, \quad (A8)
\]

where \( E(Y) \) is the expectation value of \( Y \). Define a second random variable \( X \), such that \( Y = [X - E(X)]^m \), where \( m \) is an even integer. Then,

\[
Pr \left( |X - E(X)|^m \geq \delta \right) \leq \frac{E \{ |X - E(X)|^m \}}{\epsilon^m} \quad (A9)
\]

This bound is expressed in terms of the \( m^\text{th} \) central moment of \( X \), if it exists. The result reduces to Chebyshev’s inequality for \( m = 2 \).

Note that if one treats \( b_\Theta(E) \) as a probability distribution function for a zero-mean random variable \( E \), the above inequality provides a bound for the area outside the main lobe (i.e., \( \epsilon = \Delta e \)). The central moment is evaluated for \( m = \Theta - 2 \).

\[
E \{ |X - E(X)|^m \} = \int_{-\infty}^{\infty} \Theta^{-2} b_\Theta(E) dE = \frac{\alpha_\Theta \left( \frac{\Delta e}{\pi} \right)^{\Theta - 1}}{\int_{-\infty}^{\infty} \sin \frac{\Theta x}{x^2} \, dx}
\]

\[
= \frac{\alpha_\Theta \left( \frac{\Delta e}{\pi} \right)^{\Theta - 1}}{\int_{-\infty}^{\infty} \sin^2 \frac{\Theta x}{x^2} \, dx}
\]

\[
= \frac{\alpha_\Theta \left( \frac{\Delta e}{\pi} \right)^{\Theta - 1}}{\pi} \quad (A10)
\]

If we define the area outside the main lobe as

\[
A_{\text{side}} \equiv 1 - \int_{-\Delta e}^{\Delta e} b_\Theta(E) dE, \quad (A11)
\]

then,

\[
A_{\text{side}} = Pr \left( |X - E(X)| \geq \Delta e \right) \leq \frac{\alpha_\Theta \Delta e}{\pi \Theta - 2}. \quad (A12)
\]

Combining Eq. [A12] with Lemma 1, we find

\[
A_{\text{side}} < \frac{c}{\pi \Theta - 3} \sqrt{\frac{\Theta}{6\pi}}. \quad (A13)
\]