# Efficiency of free-energy calculations of spin lattices by spectral quantum algorithms

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Ensemble quantum algorithms are well suited to calculate estimates of the energy spectra for spin-lattice systems. Based on the phase estimation algorithm, these algorithms efficiently estimate discrete Fourier coefficients of the density of states. Their efficiency 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. The dynamics of these models are specified by a Hamiltonian $\hat{\mathcal{H}}$ 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 per spin, $F$, on system parameters such as the temperature or applied magnetic field; partial derivatives of $F$ yield the thermodynamic functions. Thus, the calculation of $F$ over a wide range of parameters suffices for the determination of the finite temperature behavior of the spin-lattice model.

Calculation of the free energy for a general spin lattice by conventional means is difficult. A brute-force approach would be enumerate the eigenenergies $\{E_m\}$ of $\hat{\mathcal{H}}$, since

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

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 [1,2], histogram methods [3,4], and cumulant expansion [5,6] techniques. However, the ''sign problem'' (see, for example, Ref. [7]) prevents the 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 Eq. (1) may be written in the form

$$F=-n^{-1}k_B\theta\ln\left(\int_{-\infty}^{\infty}\rho(E)e^{-\beta E}dE\right), \qquad (2)$$

an approximation for the density of states 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 eigenvalues of Hermitian operators [8–14]. We focus on algorithms based on the phase estimation algorithm [11,12] that efficiently generate estimates of individual Fourier components $f_\ell$ of $\rho(E)$; they will be reviewed in detail in Sec. 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 in the literature is the efficiency of these algorithms for calculating thermodynamic functions. 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

$$\mathrm{Prob}(|\tilde{F}'-F|<\gamma k_B\theta)>1-\epsilon, \qquad (3)$$

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 1.

We examine the primary sources of error involved in the calculation of $\tilde{F}'$ 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. We denote an estimate of the free energy per spin subject to this broadening error by $F'$. Second, there is an inherent *stochastic* source of error reflected in the deviations in the estimated $f_\ell$ from their actual values. Subject to both deterministic and stochastic errors, an estimate of the free energy per spin is labeled $\tilde{F}'$.

In this paper, we will show that if the $f_\ell$ are known exactly, the bound in Eq. (3) may be met by a function that scales polynomially with $n$. Thus, the deterministic error due

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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).

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 $\tilde{F}'$ from the Fourier components and discusses the influence of sampling and window functions. In Sec. IV, we analyze the deterministic error due to broadening and determine the number of samples required to satisfy Eq. (3). In Sec. 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 first describe a simple algorithm applicable only to Hamiltonians that are diagonal in the computational basis, and then discuss a more general algorithm [15] applicable to ensemble quantum computers.

As regards 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 $\hat{\sigma}_z^{(j)}$ Pauli spin operator with eigenvalues $\pm 1$. The computational basis states for the quantum computer are denoted as $|x\rangle=|x_1\rangle_1|x_2\rangle_2\cdots|x_p\rangle_p$, 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 $\hat{\sigma}_z^{(j)}$ in the spin system to the logical $|0\rangle_j$ and $|1\rangle_j$ states of qubit $j$ of the quantum computer. Note that this restriction does not preclude the treatment of lattices of particles with spins larger than 1/2. Generalized Jordan-Wigner transformations exist [16,17] 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 physical interest. As an example, consider a lattice of particles interacting by an nearest-neighbor $XXZ$ interaction:

$$\hat{\mathcal{H}}=\sum_{\langle i,j\rangle}\left[J_x(\hat{\sigma}_x^{(i)}\hat{\sigma}_x^{(j)}+\hat{\sigma}_y^{(i)}\hat{\sigma}_y^{(j)})+J_z\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right]. \tag{4}$$

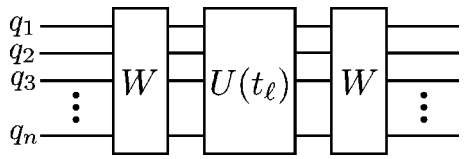


FIG. 1. Logic diagram of an elementary algorithm to estimate $|g_\ell|$.

The expectation value of the summand in Eq. (4) must lie between $-(2|J_x|+|J_z|)$ and $(2|J_x|+|J_z|)$. The energy bandwidth is bounded by the product of this constant and the number of interacting pairs in the lattice, which is a function linear in $n$. By similar reasoning, for any Hamiltonian involving only pairwise interactions between spins (of $n$-independent interaction energy), the energy bandwidth is $O(n^2)$ [22].

Second, we assume that the time-evolution operator $\hat{U}(t)\equiv\exp(-i\hat{\mathcal{H}}t)$ 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 pairwise interactions (e.g., the Ising model), this decomposition is elementary. Otherwise, one may use a Trotter-Suzuki expansion of non-commuting terms to implement $\hat{U}(t)$ to arbitrarily small error [18,19].

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:

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

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

$$g(t)\equiv\frac{f(t)}{2^n}=\frac{1}{2^n}\mathrm{Tr}(e^{-i\hat{\mathcal{H}}t}) \tag{6}$$

such that $|g(t)|\leqslant 1$. The algorithms described in this section, based on Kitaev's algorithm [9] and the phase estimation algorithm [11,12], 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 $\hat{\mathcal{H}}$ is diagonal in the computational basis. As an example, one might consider a nearest-neighbor Ising model in a longitudinal magnetic field:

$$\hat{\mathcal{H}}=J_z\sum_{\{i,j\}}(1-\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)})+h\sum_i(1-\hat{\sigma}_z^{(i)}). \tag{7}$$

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

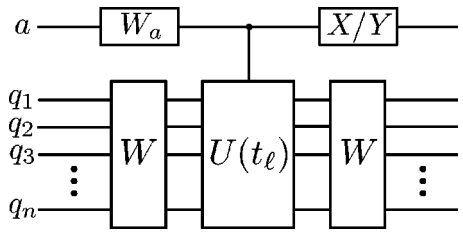


FIG. 2. Logic diagram of an algorithm to estimate the real and imaginary parts of $g_\ell$ for diagonal $\hat{\mathcal{H}}$.

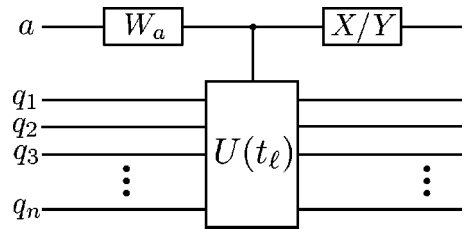


FIG. 3. Logic diagram of an ensemble algorithm to estimate $g_\ell$ for arbitrary $\hat{\mathcal{H}}$.

computer is initialized to the $|0\rangle$ state. The gate $W$ corresponds to a sequence of Walsh-Hadamard gates $W_j$ for each qubit $j$,

$$W_j:\begin{cases} |0\rangle_j \rightarrow \frac{1}{\sqrt{2}}(|0\rangle_j + |1\rangle_j) \\ |1\rangle_j \rightarrow \frac{1}{\sqrt{2}}(|0\rangle_j - |1\rangle_j). \end{cases} \tag{8}$$

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 $|g_\ell|^2$:

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

$$\xrightarrow{W} g_\ell |0\rangle + \text{orthogonal components}. \tag{9}$$

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, 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 $X \equiv \exp(i\pi\hat{\sigma}_x^{(a)}/4)$ and $Y \equiv \exp(i\pi\hat{\sigma}_y^{(a)}/4)$ gates correspond to $\pi/2$ rotations of the ancilla qubit. If the $X$ gate is used, the probabilities of observing the $|\phi_0\rangle \equiv |0\rangle_a |0\rangle_{q_1} \cdots |0\rangle_{q_n}$ or $|\phi_1\rangle \equiv |1\rangle_a |0\rangle_{q_1} \cdots |0\rangle_{q_n}$ states are

$$p_{X0} = \left|\frac{1+ig_\ell}{2}\right|^2, \quad p_{X1} = \left|\frac{1-ig_\ell}{2}\right|^2, \tag{10}$$

respectively. The $Y$ gate leads to probabilities

$$p_{Y0} = \left|\frac{1+g_\ell}{2}\right|^2, \quad p_{Y1} = \left|\frac{1-g_\ell}{2}\right|^2. \tag{11}$$

By executing $R$ iterations of the algorithm with the $X$ gate and $R$ iterations with the $Y$ gate, one can derive estimators $\tilde{p}$ for the probabilities. Unbiased estimates of the real and imaginary parts of $g_\ell$ are

$$\mathrm{Re}(\tilde{g}_\ell) = (\tilde{p}_{Y0} - \tilde{p}_{Y1}), \tag{12}$$

$$\mathrm{Im}(\tilde{g}_\ell) = (\tilde{p}_{X1} - \tilde{p}_{X0}). \tag{13}$$

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 the eigenstates of $\hat{\mathcal{H}}$; hence the restriction to Hamiltonians that are diagonal in the computational basis. One may instead consider 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 fully mixed state [15]. The initial density matrix for the system is

$$\hat{\rho}_i = \frac{1}{2^{n+1}} (\hat{I}^{(a)} + \hat{\sigma}_z^{(a)}) \hat{I}^{(q_1)} \hat{I}^{(q_2)} \cdots \hat{I}^{(q_n)}, \tag{14}$$

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 $\Sigma_\ell |\psi_\ell\rangle\langle\psi_\ell|$, where $\{|\psi_\ell\rangle\}$ is an orthogonal set of states in the subspace spanned by qubits $q_1$ to $q_n$. One could use as $\{|\psi_\ell\rangle\}$ the eigenstates of the Hamiltonian $\hat{\mathcal{H}}$. We do not need to explicitly solve for these eigenstates; the initial density matrix can be considered as an incoherent mixture of eigenstates for any Hamiltonian $\hat{\mathcal{H}}$.

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

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

$$\langle \hat{\sigma}_z^{(a)} \rangle = \mathrm{Im}(g_\ell), \tag{15}$$

whereas the $Y$ gate leads to

$$\langle \hat{\sigma}_z^{(a)} \rangle = \mathrm{Re}(g_\ell). \tag{16}$$

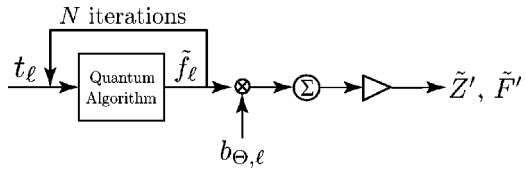


FIG. 4. Block diagram of the calculation of $\tilde{F}'$.

Thus, the real and imaginary components of the estimator $\tilde{g}_\ell$ can be calculated from two iterations of the ensemble quantum algorithm.

The ensemble algorithm is interesting for two reasons. First, it is applicable to any spin-1/2 lattice Hamiltonian $\hat{\mathcal{H}}$, provided that the time-evolution operator can be decomposed into a sufficiently small number of 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 well approximated by the identity operator. One pseudopure-state qubit can be created from two thermal spins [20].

## III. FREE-ENERGY ESTIMATION

In this section, we discuss how an estimate $\tilde{F}'$ of the free energy is generated from the Fourier components of the density of states, and examine the effects of discretization on the estimated density of states.

A conceptual overview of the free energy calculation including post-processing is shown in Fig. 4. $N$ samples of $f(t)$ are estimated via the quantum algorithm [23], and are weighted by a windowing function $b_\Theta(t)$, described below. Fourier transformation yields an estimate for the density of states, which may be integrated to compute the partition function and, thus, the free energy.

Let us first leave aside the consideration of stochastic sources of error. As iterations of the quantum algorithm yield discrete samples of $f(t)$, the reconstructed estimate $\rho'(E)$ is distorted relative to the exact density of states. Any quantity calculated from discretized Fourier components will be labeled by a prime [i.e., $\rho'(E)$]. The distortion in the density of states translates into error in $F'$. It is convenient to view this error in the context of the 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 $b_1(t)$ that is constant for $|t|\leqslant T_0/2$ and zero elsewhere] leads to a convolution of the density of states with a broadening function $b_1(E)\equiv\alpha_1\mathrm{sinc}(\pi E/\Delta e)$ $=\alpha_1[\sin(\pi E/\Delta e)]/(\pi E/\Delta e)$, where the energy resolution $\Delta e$ is given by

$$\Delta e=\frac{2\pi}{T_0}. \tag{17}$$

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 $F'$.

The effect of sampling on the estimated density of states can be determined by multiplying $f(t)b_1(t)$ by an impulse train $s(t)$ of spacing $\Delta t$:

$$s(t)=\Delta t\sum_{\ell=-\infty}^{\infty}\delta(t-\ell\Delta t). \tag{18}$$

Sampling leads to periodic replication of the broadened density of states. The resultant function is given by the Fourier transform of $f(t)b_1(t)s(t)$:

$$\rho'(E)\equiv\rho(E)*b_1(E)*\sum_{k=-\infty}^{\infty}\delta\left(E+\frac{2\pi k}{\Delta t}\right), \tag{19}$$

where the asterisk denotes convolution.

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

$$\Delta t\leqslant\frac{2\pi}{\Delta E}. \tag{20}$$

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, in which case the equality in Eq. (20) holds.

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. (3) 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 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

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

which exhibits a $1/E^\Theta$ envelope. The value of $\alpha_\Theta$ is determined by constraining the area under $b_\Theta(E)$ to equal 1. In practice, a given window shape is constructed by obtaining samples $f_\ell$ within the window width $\Theta T_0$ centered at $t=0$, and weighting each sample by $b_{\Theta,\ell}\equiv b_\Theta(t_\ell)$.

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 trade-off 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 $Z'$ for the partition function can be calculated directly from the estimated Fourier components without intermediate calculation of the density of states. The Fourier transform of $f(t)b_\Theta(t)s(t)$ may be evaluated explicitly via Eq. (18) to give an estimate $\rho'(E)$ of the broadened, periodically replicated density of states in terms of the components $f_\ell$:

$$\begin{aligned}\rho'(E)&=\frac{1}{2\pi}\int_{-\infty}^{\infty}f(t)b_\Theta(t)\left[\Delta t\sum_{\ell=-\infty}^{\infty}\delta(t-\ell\Delta t)\right]e^{iEt}dt\\&=\frac{\Delta t}{2\pi}\sum_{\{t_\ell\}}f_\ell b_{\Theta,\ell}e^{iEt_\ell},\end{aligned} \tag{23}$$

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, using Eqs. (6) and (20), and labeling quantities with a tilde to acknowledge stochastic errors, one finds

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

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 stochastic 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. (3). At this point, we consider the individual samples of $g_\ell$ to be known exactly (allowing us to omit the tilde over all quantities), and only consider the error in $F'$ due to the finite number of Fourier components—i.e., due only to the 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 $Z'$. As

$$|F'-F|<\gamma k_B\theta\Leftrightarrow e^{-\gamma n}-1<\frac{Z'-Z}{Z}<e^{\gamma n}-1, \tag{25}$$

it is sufficient to demand that

$$\mathrm{Prob}\left(r\equiv\left|\frac{Z'-Z}{Z}\right|<\xi\right)>1-\epsilon, \tag{26}$$

where $\xi\equiv1-\exp(-\gamma n)=O(n)$. In other words, satisfaction of Eq. (26) automatically implies Eq. (3).

From 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 $c\approx2.0367$.

*Lemma 2.*

$$A_{\mathrm{side}}\equiv1-\int_{-\Delta e}^{\Delta e}b_\Theta(E)dE<\frac{c}{\pi^{\Theta-3}}\sqrt{\frac{\Theta}{6\pi}}, \tag{29}$$

where $\Theta$ is an even integer.

Lemma 1 places an upper bound on $\alpha_\Theta$ such that $b_\Theta(E)$ is normalized. Lemma 2 defines 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); this bound decreases exponentially with $\Theta$. Both lemmas are proved in the Appendix.

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) and (20) evaluated at the Nyquist condition yield

$$\begin{aligned}Z'&=\int_0^{\Delta E}\rho'(E)e^{-\beta E}dE\\&=\sum_m\sum_{k=-\infty}^{\infty}\int_0^{\Delta E}b_\Theta(E-E_m+k\Delta E)e^{-\beta E}dE\\&=\sum_m\left[\sum_{k=-\infty}^{\infty}\int_{k\Delta E}^{(k+1)\Delta E}b_\Theta(E-E_m)e^{-\beta(E-k\Delta E)}dE\right]\\&\equiv\sum_m Z'_m.\end{aligned} \tag{30}$$

The change of variables allows one to view $Z'_m$ as an integral of the broadening function, centered at $E_m$, and weighted by periodically replicated segments of an exponential function. $Z'$ is found by summing over all eigenenergies.

The maximum relative error $r$ in the partition function is bounded by the largest contribution from any single eigenenergy, which we define as $r_m \equiv \max_m |(Z'_m - Z_m)/Z_m|$, where $Z_m \equiv e^{-\beta E_m}$. Defining $\gamma_m = Z'_m/Z_m$, it follows that

$$r = \left| \frac{Z' - Z}{Z} \right| = \frac{\left| \sum_m (Z'_m - Z_m) \right|}{\sum_m Z_m} = \frac{\left| \sum_m (\gamma_m - 1) Z_m \right|}{\sum_m Z_m}$$

$$\leqslant \max_m |\gamma_m - 1| = \max_m \left| \frac{Z'_m - Z_m}{Z_m} \right| = r_m . \quad (31)$$

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 $r_m$ for this simplified system at any $E_m$ suffices to bound the error for an arbitrary energy spectrum over the same bandwidth.

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

$$r_m < \max\left( \left| \frac{Z'_{m,\min} - Z_m}{Z_m} \right|, \left| \frac{Z'_{m,\max} - Z_m}{Z_m} \right| \right). \quad (32)$$

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,

$$Z'_m = \sum_{k=-\infty}^{\infty} \int_{k\Delta E}^{(k+1)\Delta E} b_\Theta(E - E_m) e^{-\beta(E - k\Delta E)} dE$$

$$\geqslant (1 - A_{\text{side}}) e^{-\beta(E_m + \Delta e)} + A_{\text{side}} e^{-\beta \Delta E} \equiv Z'_{m,\min}. \quad (33)$$

Similarly, as the maximum value of the Boltzmann factor is $e^{-\beta(E_m - \Delta e)}$ inside the main lobe and 1 outside,

$$Z'_m \leqslant (1 - A_{\text{side}}) e^{-\beta(E_m - \Delta e)} + A_{\text{side}} \equiv Z'_{m,\max}. \quad (34)$$

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

$$r_m < \max[\, 1 - (1 - A_{\text{side}}) e^{-\beta \Delta e} - A_{\text{side}} e^{-\beta(\Delta E - E_m)},$$

$$(1 - A_{\text{side}}) e^{\beta \Delta e} + A_{\text{side}} e^{\beta E_m} - 1 \,]. \quad (35)$$

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

$$\beta \Delta e = \ln(1 + \xi/2), \quad (36)$$

$$A_{\text{side}} < \frac{\xi}{2} e^{-\beta \Delta E}. \quad (37)$$

As proof of their sufficiency, note that

$$1 - (1 - A_{\text{side}}) e^{-\beta \Delta e} - A_{\text{side}} e^{-\beta(\Delta E - E_m)}$$

$$< \frac{\xi}{2} + \frac{\xi}{2} e^{-\beta \Delta E} \left( 1 - \frac{\xi}{2} \right) < \xi, \quad (38)$$

and

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

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

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

$$\Delta e = \frac{\ln(1 + \xi/2)}{\beta}, \quad (40)$$

$$\Theta - \frac{\ln \Theta}{2 \ln \pi} > \frac{\beta \Delta E}{\ln \pi} + \frac{\ln(1/\xi)}{\ln \pi} + \kappa, \quad (41)$$

where $\kappa = 5/2 + \ln(2c/\sqrt{6})/\ln \pi \approx 2.9443$. As $\ln \Theta < \Theta$, a sufficient condition to satisfy Eq. (41) is

$$\Theta/2 = \lceil \mu \beta \Delta E + \mu \ln(1/\xi) + \kappa' \rceil, \quad (42)$$

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

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. (40) and (42) into Eq. (27), disregarding the weak logarithmic dependence of $\Theta$ and $\Delta e$ on $n$.

$$N = \frac{\Theta \Delta E}{\Delta e} \propto \frac{(\beta \Delta E)(\Delta E)}{1/\beta} = \beta^2 (\Delta E)^2 \propto \text{poly}(n), \quad (43)$$

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

Ultimately, the precision with which the expected value of the ancilla qubit may be measured is determined by the number of ensemble members over which the measurement is averaged. Treating $\text{Re}(\tilde{g}_\ell)$ and $\text{Im}(\tilde{g}_\ell)$ as random variables, these fluctuations are modeled by their variances. We assume that the variances $\sigma_g^2$ are independent of $\ell$. In this section, the dependence of the maximum allowable value of $\sigma_g^2$ on $n$ such that Eq. (3) is maintained is derived.

Recall that $\tilde{Z}'$ represents an estimate of the partition function calculated from discrete and imprecise Fourier components of the density of states. As $\tilde{Z}'$ is a linear combination of the independent random variables $\text{Re}(\tilde{g}_\ell)$ and $\text{Im}(\tilde{g}_\ell)$, the variance of $\tilde{Z}'$ can be calculated from Eq. (24):

$$\sigma_{\tilde{Z}'}^2 = \left(\frac{2^n \sigma_g \Delta t}{\pi\beta}\right)^2 (1-e^{-\beta\Delta E})^2 \sum_{\ell>0}^{N/2} \frac{b_{\Theta,\ell}^2}{1+(t_\ell/\beta)^2}. \quad (44)$$

If we assume that $\tilde{Z}'$ is Gaussian distributed, then the probability of $\tilde{Z}'$ 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 $T_0$. In the limit of large $\Theta$, $b_\Theta(t)$ may be approximated by

$$b_\Theta(t) \approx e^{-t^2/2\nu^2}, \quad (45)$$

where $\nu^2 = \Theta T_0^2/12$ [24]. Although this approximation overestimates $b_\Theta(t)$ away from $t=0$, the fractional error in Eq. (44) incurred by the approximation is less than $5\times10^{-3}$ for $\Theta > 40$. Second, it is assumed that $\beta/\Delta t = \beta\Delta E/2\pi \gg 1$, implying that the energy bandwidth is much larger than the thermal energy. This condition assures that the sum can be well approximated by the integral

$$\sigma_{\tilde{Z}'}^2 \approx \left(\frac{2^n \sigma_g \Delta t}{\pi\beta}\right)^2 \int_0^\infty \frac{e^{-t^2/\nu^2}}{1+t^2/\beta^2} \frac{dt}{\Delta t}$$
$$= \frac{4^n \sigma_g^2}{\beta\Delta E} e^{\beta^2/\nu^2}[1-\mathrm{erf}(\beta/\nu)]. \quad (46)$$

Equation (46) indicates that the standard deviation of $\tilde{Z}'$ scales exponentially with $n$; i.e., as $2^n$ [25]. 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 $n$ noninteracting 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. (7), $Z = (1+e^{-2\beta J})^n$ for periodic boundary conditions. Thus, if the distribution function for $\tilde{Z}'$ is Gaussian, one expects that the standard deviation increases exponentially faster [26] 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. (1), the condition $|\tilde{F}'-F| < \gamma k_B \Theta$ in Eq. (3) is equivalent to

$$Ze^{-\gamma n} < \tilde{Z}' < Ze^{\gamma n}. \quad (47)$$

Assuming a Gaussian distribution for $\tilde{Z}'$ centered about $Z$,

$$\epsilon = 1 - \mathrm{Prob}(Ze^{-\gamma n} < \tilde{Z}' < Ze^{\gamma n})$$
$$= \frac{1}{2}\left\{ \mathrm{erfc}\left[\frac{Z(e^{\gamma n}-1)}{\sqrt{2}\sigma_{\tilde{Z}'}}\right] + \mathrm{erfc}\left[\frac{Z(1-e^{-\gamma n})}{\sqrt{2}\sigma_{\tilde{Z}'}}\right]\right\}. \quad (48)$$

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

$$\epsilon = \mathrm{erfc}\left(\frac{Z\gamma n}{\sqrt{2}\sigma_{\tilde{Z}'}}\right) \approx \mathrm{erfc}\left(\sqrt{\frac{\beta\Delta E}{2}}\frac{Z\gamma n}{2^n\sigma_g}\right). \quad (49)$$

The argument of the $\mathrm{erfc}(\cdot)$ function must be of order unity or larger for $\epsilon < 0.1$, so

$$\sigma_g^2 = O\left(\frac{Z^2 \mathrm{poly}(n)}{4^n}\right). \quad (50)$$

By the above argument, the variance in the measured Fourier components must decrease exponentially with $n$. Exponential precision in the calculated Fourier components is required to satisfy Eq. (3).

## VI. CONCLUSION

We examined the applicability of selected 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.

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## APPENDIX: PROOFS OF LEMMAS 1 AND 2

*Proof of Lemma 1*. A lower bound is first derived for

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

We exclude infinitesimal regions around $x = m\pi$ $(m \in \mathcal{Z})$ from the integral to avoid divergence of the logarithm; as

$\mathrm{sinc}(x)$ 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 $\ln[\mathrm{sinc}(x)]$ [21],

$$\ln[\mathrm{sinc}(x)] = -\frac{x^2}{6} - \sum_{k=2}^{\infty} \frac{x^{2k}}{k\pi^{2k}} \left( \sum_{n=1}^{\infty} \frac{1}{n^{2k}} \right) > -\frac{x^2}{6} - \left( \frac{\pi^2}{6} \right) \sum_{k=2}^{\infty} \frac{x^{2k}}{k\pi^{2k}}. \tag{A2}$$

Thus,

$$I > \int_{-\infty}^{\infty} e^{-\Theta x^2/6} \exp\left( -\frac{\Theta \pi^2}{6} \sum_{k=2}^{\infty} \frac{x^{2k}}{k\pi^{2k}} \right) dx. \tag{A3}$$

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,

$$I > \exp\left( -\frac{\Theta \pi^2}{6} \sum_{k=2}^{\infty} \frac{(6/\Theta)^k}{k\pi^{2k}} \right) \int_{-\sqrt{6/\Theta}}^{\sqrt{6/\Theta}} e^{-\Theta x^2/6} dx. \tag{A4}$$

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

$$I > e^{1+\pi^2\Theta \ln(1-6/\pi^2\Theta)/6} \sqrt{\frac{6\pi}{\Theta}} \mathrm{erf}(1) = e \left( 1 - \frac{6}{\Theta\pi^2} \right)^{\Theta\pi^2/6} \mathrm{erf}(1) \sqrt{\frac{6\pi}{\Theta}} > \left( 1 - \frac{6}{\pi^2} \right)^{\pi^2/6} \mathrm{erf}(1) \sqrt{\frac{6\pi}{\Theta}}. \tag{A5}$$

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 $\alpha_\Theta$:

$$\alpha_\Theta = \frac{1}{\int_{-\infty}^{\infty} \left[ \mathrm{sinc}\left( \frac{\pi E}{\Delta e} \right) \right]^\Theta dE} = \frac{\pi}{\Delta e\, I} < \frac{\pi}{\Delta e} \left( c \sqrt{\frac{\Theta}{6\pi}} \right), \tag{A6}$$

where $c$ is defined as

$$c \equiv \frac{1}{e} \left( \frac{1}{1-6/\pi^2} \right)^{\pi^2/6} \frac{1}{\mathrm{erf}(1)} \approx 2.0367. \tag{A7}$$

*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:

$$\Pr(Y \geq \delta) \leq \frac{E(Y)}{\delta}, \tag{A8}$$

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,

$$\Pr\{[X-E(X)]^m \geq \delta\} \leq \frac{E\{[X-E(X)]^m\}}{\delta} \Rightarrow \Pr\{|X-E(X)| \geq \epsilon\} \leq \frac{E\{[X-E(X)]^m\}}{\epsilon^m}. \tag{A9}$$

This bound is expressed in terms of the $m$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 $m = \Theta - 2$:

$$E\{[X-E(X)]^m\} = \int_{-\infty}^{\infty} E^{\Theta-2} b_\Theta(E)\, dE = \alpha_\Theta \left( \frac{\Delta e}{\pi} \right)^{\Theta-1} \int_{-\infty}^{\infty} \frac{\sin^\Theta x}{x^2} dx \leq \alpha_\Theta \left( \frac{\Delta e}{\pi} \right)^{\Theta-1} \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \alpha_\Theta \left( \frac{\Delta e}{\pi} \right)^{\Theta-1} \pi. \tag{A10}$$

If we define the area outside the main lobe as

$$A_{\mathrm{side}} \equiv 1 - \int_{-\Delta e}^{\Delta e} b_\Theta(E)\, dE, \tag{A11}$$

then

$$A_{\mathrm{side}} = \Pr\{|X-E(X)| \geq \Delta e\} \leq \frac{\alpha_\Theta \Delta e}{\pi^{\Theta-2}}. \tag{A12}$$

Combining Eq. (A12) with Lemma 1, we find

$$A_{\mathrm{side}} < \frac{c}{\pi^{\Theta-3}} \sqrt{\frac{\Theta}{6\pi}}. \tag{A13}$$

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[22] This assumption is more restrictive if a pairwise Hamiltonian for a lattice of particles with spins larger than 1/2 is transformed to an equivalent spin-1/2 lattice, as the transformed Hamiltonian will not necessarily consist of only pairwise interactions.
[23] As this section exploits the Fourier relationship between $f(t)$ and the density of states, it is more convenient notationwise to commence with the former than $g(t)$.
[24] As the Fourier transform of $b_\Theta(t)$ is the broadening function $b_\Theta(E)$, which is of unit area, $b_\Theta(t=0)=1$.
[25] Although the term $e^{\beta^2/\nu^2}[1-\mathrm{erf}(\beta/\nu)]$ is a weakly decreasing function of $n$, the $4^n$ dependence dominates.
[26] The mean of $\tilde{Z}'$ is not strictly $Z$ due to the broadening error, but may be bounded to an arbitrarily small region about $Z$ by the techniques of the preceding section.