On the representation of Boolean and real functions as Hamiltonians for quantum computing

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Abstract

Mapping functions on bits to Hamiltonians acting on qubits has many applications in quantum computing. In particular, Hamiltonians representing Boolean functions are required for applications of quantum annealing or the quantum approximate optimization algorithm to combinatorial optimization problems. We show how such functions are naturally represented by Hamiltonians given as sums of Pauli Z operators (Ising spin operators) with the terms of the sum corresponding to the function's Fourier expansion. For many classes of functions which are given by a compact description, such as a Boolean formula in conjunctive normal form that gives an instance of the satisfiability problem, it is #P-hard to compute its Hamiltonian representation. On the other hand, no such difficulty exists generally for constructing Hamiltonians representing a real function such as a sum of local Boolean clauses. We give composition rules for explicitly constructing Hamiltonians representing a wide variety of Boolean and real functions by combining Hamiltonians representing simpler clauses as building blocks. We apply our results to the construction of controlled-unitary operators, and to the special case of operators that compute function values in an ancilla qubit register. Finally, we outline several additional applications and extensions of our results.

A primary goal of this paper is to provide a *design toolkit for quantum optimization* which may be utilized by experts and practitioners alike in the construction and analysis of new quantum algorithms, and at the same time to demystify the various constructions appearing in the literature.

1 Introduction

A basic requirement of many quantum algorithms is the ability to translate between mathematical functions acting on a domain, typically a string of bits, and quantum Hamiltonian operators acting on qubits. In particular, mapping Boolean or real functions to Hamiltonians has many important applications to quantum algorithms and heuristics for solving decision problems or approximately solving optimization problems, such as quantum annealing and adiabatic quantum optimization (AQO) [1–3], or the quantum approximate optimization algorithm and the quantum alternating operator ansatz (QAOA) [4, 5], or the related variational quantum eigensolver (VQE) [6]. Explicit Hamiltonian constructions for the application of these algorithms to a variety of important decision and optimization problems can be found in [5, 7]. These quantum algorithms are promising, in particular, as possible paths towards performing truly useful computation on near-term quantum computing devices. Indeed, decision and optimization problems are ubiquitous across science and engineering, yet often appear to be computationally difficult. Despite years of investigation, efficient algorithms for these problems remain elusive [8, 9]. Hence, the potential for new approaches to tackling these problems on quantum computers is an exciting development.

Nevertheless, the conceptual barrier to entry to studying these quantum algorithms and providing new insights remains high, especially for practitioners in the domain where a given problem arises, who may not be familiar with quantum computing beyond the basics. It is thus important to develop tools and methodologies which are accessible to scientists and researchers from different domains, and are as independent of knowing the low-level details of quantum computing as possible, towards enabling easier cross-fertilization of different

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ideas and techniques and hopefully leading to new effective quantum algorithms. At the same time, it useful to provide a rigorous general foundation for existing constructions and tools found in the literature, often in a specific context. Thus, our primary goal is to provide a *design toolkit* of basic results which can be used by experts or laymen alike to design, implement, and analyze quantum algorithms for hard (classical) decision and optimization problems.

In this paper we show a general theory of mappings of Boolean and real functions to diagonal Hamiltonians acting on qubits, and give simple rules for the explicit construction of these Hamiltonians which include many typical classes of such functions such as Boolean formulas and circuits. We also address the question of when such Hamiltonians may be constructed efficiently. We then show how our results may be applied to the construction of unitary or Hermitian operators controlled by Boolean predicates, which are used, for example, in several of the QAOA mixing operator constructions in [5]. Our results are general and give a methodical approach to derive many of the mappings in the literature such as those of [5, 7]. We emphasize that our results have applications to quantum algorithms beyond quantum annealing or QAOA, and we outline several additional applications including subspace encodings and oracle queries.

We elaborate on our results, which we summarize in the next section. Consider a function f acting on n bits. We say a Hamiltonian H_f *represents* f if it satisfies

$$H_f|x\rangle = f(x)|x\rangle \tag{1}$$

for each input string $x \in \{0,1\}^n$ with corresponding computational basis state $|x\rangle$. We show how arbitrary n-bit Boolean or real functions are naturally represented as diagonal Hamiltonians given by weighted sums of Pauli Z operators, with terms corresponding to the function's Fourier expansion, as summarized in Propostion 1 below. Such Hamiltonians generalize the Ising model of interacting spin-1/2 particles common in physics. Our results rely on the Fourier analysis of Boolean functions, which has many well-known applications in computer science [10–13], and in particular quantum computation [14, 15]. Next, we derive the explicit Hamiltonian representations of basic Boolean predicates. The properties of the Fourier expansion then lead to composition rules for constructing Hamiltonians representing conjunctions, disjunctions, exclusive or, and other functions of simpler clauses by combining their Hamiltonian representations in particular ways (see Theorem 1 below). Furthermore, these mappings extend to directly constructing Hamiltonians representing weighted sums of clauses, which are a primary class of Hamiltonians considered in quantum annealing and QAOA, for example, for solving constraint satisfaction problems.

We also consider the computational complexity of such Hamiltonian constructions, which naturally depends on how the function f is provided as input. Many combinatoric properties of a given function can be "read off" from its Fourier coefficients [16]. This presents an obstruction to computing the Hamiltonian representation for general Boolean functions; we show that computing the identity component of $H_f = \widehat{f}(\emptyset)I + \dots$, which is given by the first Fourier coefficient $\widehat{f}(\emptyset)$ of f, is as hard as counting the the number of inputs such that $f = 1$, which in general is computationally intractable. For example, if f is a Boolean formula on n variables given in conjunctive formula form with a poly(n) size description, i.e., an instance of the satisfiability problem (SAT), then this is #P-hard so it is not believed possible to efficiently compute $\widehat{f}(\emptyset)$; if such a classical polynomial-time algorithm existed then we would have P=NP. Hence, we cannot efficiently construct explicit Hamiltonian representations of many n-bit Boolean functions, even when such a function is described by only poly(n) bits.

Nevertheless, there is no such difficulty for *local* Boolean functions f_j where each f_j acts on a constant number of bits. This allows us to efficiently construct Hamiltonians representing *pseudo-Boolean* functions of the form $f(x) = \sum_{j=1}^m f_j(x)$, $m = \text{poly}(n)$. Such real functions (and their corresponding Hamiltonians) may be constructed such that their minimum value solution (lowest eigenvalue eigenvector, i.e., ground state) encodes the solution to a corresponding decision problem; similar to, for example, how solving the MAX-SAT problem (finding the maximum possible number of satisfied clauses) also solves SAT. For a pseudo-Boolean function, in general its Fourier coefficients do not explicitly encode its optimal value, so its Hamiltonian representation can often be computed efficiently. Indeed, this is a common approach to encoding decision problems such as SAT into the framework of quantum annealing [7].

1.1 Main Results: A Design Toolkit for Quantum Optimization Algorithms

We now give our main results. Representing Boolean and real (pseudo-Boolean) functions as Hamiltonians is addressed in detail in Section 2. We extend our results to controlled unitaries and operators computing

functions in ancilla registers in Section 3. Finally, we outline several additional applications of our results as an appendix.

1.1.1 Boolean Functions

Boolean functions can be represented as diagonal Hamiltonians. We show how every such function naturally maps to a Hamiltonian expressed as a linear combination of Pauli Z operators, with terms corresponding to the Fourier expansion of the function. For the (faithful) representation on n qubits, this mapping is unique.

Proposition 1. *For a Boolean function $f : \{0,1\}^n \to \{0,1\}$, the unique Hamiltonian on n-qubits satisfying $H_f|x\rangle = f(x)|x\rangle$ for each computational basis state $|x\rangle$ is*

$$
\begin{aligned}
H_f &= \sum_{S \subset [n]} \widehat{f}(S) \prod_{j \in S} Z_j \\
&= \widehat{f}(\emptyset)I + \sum_{j=1}^{n} \widehat{f}(\{j\})Z_j + \sum_{j<k} \widehat{f}(\{j,k\})Z_j Z_k + \dots
\end{aligned} \tag{2}
$$

where the Fourier coefficients $\widehat{f}(S) = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x)(-1)^{S \cdot x}$ satisfy

$$
\sum_{S \subset [n]} \widehat{f}(S)^2 = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x) = \widehat{f}(\emptyset). \tag{3}
$$

Here we have used the notation $S \cdot x := \sum_{j \in S} x_j$, $[n] = \{1, 2, \dots, n\}$, and Z_j denotes the Z operator applied to the jth qubit. The proposition follows from Theorem 2 which is given in Section 2.

Thus, computing the Hamiltonian representation (2) of a Boolean function is equivalent to computing its Fourier expansion. By considering a Boolean function corresponding to an NP-hard decision problems (more precisely, a function corresponding to a #P-hard counting problem), from (3) we have the following corollary.

Corollary 1. *Computing the identity coefficient $\widehat{f}(\emptyset)$ of the Hamiltonian H_f representing a Boolean satisfiability (SAT) formula f (given in conjunctive normal form) is #P-hard. Deciding if $\widehat{f}(\emptyset) = 0$ is equivalent to deciding if f is unsatisfiable, in which case H_f is identically (reducible to) the 0 matrix.*

Hence, for any Boolean function f given in a form such that counting its number of satisfying inputs is #P-hard, computing the identity coefficient $\widehat{f}(\emptyset)$ of its Hamiltonian representation will be #P-hard also. Such hard counting problems include not only functions corresponding to NP-hard decision problems such as SAT, but also certain functions corresponding to decision problems decidable in polynomial time, such as counting the number of perfect matchings in a bipartite graph; see e.g. [9]. Note that the quantity $\widehat{f}(\emptyset)$ is proportional to the trace of H_f and hence is basis independent.

We emphasize that even if we could, somehow, compute the value of each Fourier coefficient, a Hamiltonian H_f representing a general Boolean function on n bits may require a number of Pauli Z terms that are exponentially many with respect to n. We define the size of H_f, size(H_f), to be the number of nonzero terms in the sum (2), and the degree of H_f, deg(H_f) = deg(f), to be the maximum locality (number of qubits acted on) of any such term. Hence, we consider a family of n-bit functions f_n to be *efficiently representable* as the Hamiltonians H_{f_n} if size(H_{f_n}) grows polynomially with n for each f_n and so does the cost for computing each of the nonzero coefficients.[1]

1.1.2 Constructing Hamiltonians

The construction of Hamiltonians representing standard Boolean functions follows directly from Proposition 1. We summarize mappings of some important basic clauses in Table 1 below.

We show formal rules for combining Hamiltonians representing different Boolean functions to obtain Hamiltonians representing more complicated expressions involving these functions. In particular, we consider the logical negation($\neg$), conjunction ($\wedge$), disjunction ($\vee$), exclusive or ($\oplus$), and implication ($\Rightarrow$) operations, and addition or multiplication by a real number when Boolean functions are taken as a subset of the real functions.

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[1]Note that we implicitly assume each f_n is described (as input) by poly(n) bits. On the other hand, if, say, each f_n is described with a number of bits that is $\Omega(2^n)$, then we may always construct H_{f_n} efficiently with respect to this exponentially large input.

$f(x)$	H_f	$f(x)$	H_f
x	$\frac{1}{2}I - \frac{1}{2}Z$	$\overline{x}$	$\frac{1}{2}I + \frac{1}{2}Z$
$x_1 \oplus x_2$	$\frac{1}{2}I - \frac{1}{2}Z_1 Z_2$	$\bigoplus_{j=1}^{k} x_j$	$\frac{1}{2}I - \frac{1}{2}Z_1 Z_2 \ldots Z_k$
$x_1 \wedge x_2$	$\frac{1}{4}I - \frac{1}{4}(Z_1 + Z_2 - Z_1 Z_2)$	$\bigwedge_{j=1}^{k} x_j$	$\frac{1}{2^k}\prod_j (I - Z_j)$
$x_1 \vee x_2$	$\frac{3}{4}I - \frac{1}{4}(Z_1 + Z_2 + Z_1 Z_2)$	$\bigvee_{j=1}^{k} x_j$	$I - \frac{1}{2^k}\prod_j (I + Z_j)$
$\overline{x_1 x_2}$	$\frac{3}{4}I + \frac{1}{4}(Z_1 + Z_2 - Z_1 Z_2)$	$x_1 \Rightarrow x_2$	$\frac{3}{4}I + \frac{1}{4}(Z_1 - Z_2 + Z_1 Z_2)$

Table 1: Hamiltonians representing basic Boolean clauses.

Theorem 1 (Composition rules). *Let f, g be Boolean functions represented by Hamiltonians H_f, H_g. Then the Hamiltonians representing basic operations on f and g are given by*

$$H_{\neg f} = H_{\overline{f}} = I - H_f \qquad\qquad H_{f \Rightarrow g} = I - H_f + H_f H_g$$

$$H_{f \wedge g} = H_{fg} = H_f H_g \qquad\qquad H_{f \vee g} = H_f + H_g - H_f H_g$$

$$H_{f \oplus g} = H_f + H_g - 2 H_f H_g \qquad\qquad H_{af+bg} = a H_f + b H_g \quad a, b \in \mathbb{R}.$$

Combining the composition rules and the results for basic clauses, Hamiltonians for a large variety of functions can be easily constructed, in particular Hamiltonians representing Boolean formulas and circuits.

1.1.3   Pseudo-Boolean functions

Consider a real function f given as a weighted sum of Boolean functions f_j,

$$f(x) = \sum_{j=1}^{m} w_j f_j(x) \qquad w_j \in \mathbb{R},$$

where f acts on n bits, and in the applications we consider often $m = \text{poly}(n)$. The objective functions for constraint satisfaction problems, considered in QAOA, are often expressed in this form, with each f_j given by a Boolean expression. A different example is the penalty term approach of quantum annealing, where the objective function is augmented with a number of high-weight penalty terms which perform (typically, local) checks to see if a state is valid; see Appendix A.1 for a discussion. For such *pseudo-Boolean functions* we have the following result.

Proposition 2. *For an n-bit real function f given as $f(x) = \sum_{j=1}^{m} w_j f_j(x)$, $w_j \in \mathbb{R}$, where the f_j are Boolean functions, the unique Hamiltonian on n-qubits satisfying $H_f |x\rangle = f(x)|x\rangle$ is*

$$H_f = \sum_{S \subset [n]} \widehat{f}(S) \prod_{j \in S} Z_j = \sum_{j=1}^{m} w_j H_{f_j}, \qquad (4)$$

with Fourier coefficients $\widehat{f}(S) = \frac{1}{2^n}\sum_{x \in \{0,1\}^n} f(x)(-1)^{S \cdot x} = \sum_j \widehat{f_j}(S) \in \mathbb{R}$, where H_{f_j} are defined as in (2).
In particular, $\deg(H_f) = \max_j \deg(f_j)$ and $\text{size}(H_f) \leq \sum_j \text{size}(H_{f_j})$.

As the terms in the Hamiltonian (4) mutually commute, we can *simulate* such an H_f, i.e., implement the operator $U = exp(-iH_f t)$ for some fixed $t \in \mathbb{R}$, using $O(\deg(H_f) \cdot \text{size}(H_f))$ many basic quantum gates (consisting of CNOT gates and Z-rotation gates $R_Z(\theta) = exp(-iZ\theta/2)$). See, e.g., [17] for standard sets of quantum gates and their details.

Note that we do not deal explicitly with issues of how the real numbers w_j may be represented and stored. For many applications, these weights are simple bounded rational numbers and this issue is relatively minor; see, e.g., the constructions in [5].

The remaining two items of the section demonstrate how our results may be applied to the construction of more general (non-diagonal) Hamiltonians and unitary operators.

1.1.4 Controlled Unitaries and Hamiltonians

In many applications we require controlled Hamiltonian simulations. Consider two quantum registers of $k + n$ qubits. Given a k-bit Boolean function $f(y)$ and a unitary operator U acting on n-qubits, we define the $(k + n)$-qubit f-controlled unitary operator $\Lambda_f(U)$ by its action on basis states

$$\Lambda_f(U)|y\rangle|x\rangle = \begin{cases} |y\rangle|x\rangle & f(y) = 0 \\ |y\rangle U|x\rangle & f(y) = 1. \end{cases}$$

Equivalently, as $H_f + H_{\overline{f}} = I$ we have the useful decomposition

$$\Lambda_f(U) = H_f \otimes U + H_{\overline{f}} \otimes I. \tag{5}$$

If U is self-adjoint, then $\Lambda_f(U)$ is also a Hamiltonian. When U is given as a time evolution under a Hamiltonian H for a time t, we have the following.

Proposition 3. *Let f be a Boolean function represented by a k-qubit Hamiltonian H_f, and let H be an arbitrary Hamiltonian acting on n disjoint qubits. Then the $(k + n)$-qubit Hamiltonian*

$$\widetilde{H}_f = H_f \otimes H \tag{6}$$

corresponds to f-controlled evolution under H, i.e., satisfies $e^{-i\widetilde{H}_f t} = \Lambda_f(e^{-iHt})$.

The proof follows from from exponentiating (6) directly. This result was used in [5] to construct controlled mixing operators $\Lambda_f(e^{-iHt})$ for QAOA mappings of optimization problems with feasibility constraints, with the important property of restricting the quantum evolution to the subspace of feasible states. In particular, operators in [5] implement evolution under local mixing Hamiltonians controlled by Boolean functions, where the control function checks for each basis state that the action of the mixing Hamiltonian will maintain state feasibility, and only applies each mixing Hamiltonian when this is the case.

1.1.5 Computing Boolean functions in registers

We show how our results may be further applied to construct explicit unitary operators (i.e., *oracle queries*) which compute function values in an ancilla qubit register.

Recall that in the computational basis, the Pauli X operator acts as $X|0\rangle = |1\rangle$ and $X|1\rangle = |0\rangle$, i.e., as the *bit-flip*, or NOT, operation.

Proposition 4. *For an n-bit Boolean function f represented by a Hamiltonian H_f, let G_f be the unitary self-adjoint operator on $n + 1$ qubits which acts on basis states $|x\rangle|a\rangle$ as*

$$G_f|x\rangle|a\rangle = |x\rangle|a \oplus f(x)\rangle.$$

Then

$$G_f = \Lambda_f(X) = e^{-i\frac{\pi}{2} H_f \otimes (X-I)}, \tag{7}$$

and $G_f = I$ if and only if f is unsatisfiable.

In particular, if f is given as a SAT formula in conjunctive normal form, then it is #P-hard to compute the identity coefficient $\widehat{g}(\emptyset) = \mathrm{tr}(G_f)/2^n$ of G_f, and NP-hard to decide if $\widehat{g}(\emptyset) \neq 1$.

With the previous results, the right-hand side of equation (7) shows how Hamiltonian simulation may be used to compute a function f in a register. In particular, as the Pauli terms in H_f mutually commute, G_f can in principle be implemented with $2 \cdot \mathrm{size}(H_f)$ many multiqubit Pauli rotations with locality up to $\deg(H_f) + 1$.

2 Representing n-bit Functions as Diagonal Hamiltonians

Many important problems and algorithms naturally involve Boolean predicates. We show how the natural representation of a Boolean function as a Hamiltonian composed of spin operators (Pauli Z matrices) follows from its Fourier expansions. Indeed, Fourier analysis of Boolean functions has many applications in theoretical computer science [10–13, 18], and is also a particularly useful tool for quantum computation [14, 15]; see [16, 19] for overviews of the subject. We further use these tools to extend our results to Hamiltonians representing more general functions built from sums, conjunctions, disjunctions, and other basic combinations of simpler Boolean clauses.

2.1 Boolean Functions

The class of Boolean functions on n bits is defined as $\mathcal{B}_n := \{f : \{0,1\}^n \to \{0,1\}\}$. As vector spaces (over $\mathbb{R}$), for each n they give a basis for the real functions on n bits, $\mathcal{R}_n = \{f : \{0,1\}^n \to \mathbb{R}\}$. Moreover, $\mathcal{R}_n$ is isomorphic to the vector space of diagonal Hamiltonians acting on n-qubits, or, equivalently, the space of $2^n \times 2^n$ diagonal real matrices. Thus, diagonal Hamiltonians naturally encode large classes of functions.

We say a Hamiltonian *represents* a function f if in the computational basis it acts as the corresponding multiplication operator, i.e., it satisfies the eigenvalue equations

$$\forall x \in \{0,1\}^n \quad H_f|x\rangle = f(x)|x\rangle. \tag{8}$$

On n qubits, this condition specifies H_f uniquely, up to the choice of the computational basis. Equivalently, we may write $H_f = \sum_x f(x)|x\rangle\langle x|$, which in the case of Boolean functions $f \in \mathcal{B}_n$ becomes

$$H_f = \sum_{x:f(x)=1} |x\rangle\langle x|. \tag{9}$$

As Boolean functions are idempotent, both $f^2 = f$ and $H_f^2 = H_f$, so H_f is a projector[2] of rank $r = \#f := |\{x : f(x) = 1\}| = \sum_x f(x)$. Hence, the Hamiltonian H_f for a Boolean function f is equivalent to the projector onto the subspace spanned by basis vectors $|x\rangle$ such that $x = 1$, and given an f describing such a subspace the corresponding projector may be constructed using our results below. Hence, determining if f is satisfiable is equivalent to determining if H_f is not identically 0, and determining H_f explicitly in the form of (9) is at least as hard as counting the number of satisfying assignments of f, or equivalently, computing $r = \text{rank}(H_f)$.

We consider the standard computational basis of eigenstates of Pauli Z operators (often written as σ_z), defined by the relations $Z|0\rangle = |0\rangle$ and $Z|1\rangle = -|1\rangle$. We use $Z_j = I \otimes \ldots I \otimes Z \otimes I \cdots \otimes I$ to denote Z acting on the jth qubit. Products of Z_j over a set of qubits act as

$$\prod_{j \in S} Z_j|x\rangle = \chi_S(x)|x\rangle, \tag{10}$$

where each *parity function* $\chi_S(x) : \{0,1\}^n \to \{-1,+1\}$ gives the parity of the bits of x in the subset $S \subset [n]$, i.e., is $+1$ if and only if the number of bits of x set to 1 is even. Identifying each S with its characteristic vector $S \in \{0,1\}^n$ such that $S \cdot x = \sum_{j \in S} x_j$, we have

$$\chi_S(x) = (-1)^{S \cdot x} = (-1)^{\oplus_{j \in S} x_j}. \tag{11}$$

Thus, each Hamiltonian $Z_S := \prod_{j \in S} Z_j$ represents the function $\chi_S(x)$ in the sense of (8).

The set of parity functions on n-bits $\{\chi_S(x) : S \subset \{0,1\}^n\}$ also gives a basis for the real functions $\mathcal{R}_n$. This basis is orthonormal with respect to the inner product defined by

$$\langle f, g \rangle := \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x)g(x). \tag{12}$$

Hence, every Boolean function $f \in \mathcal{B}_n$ may be written uniquely as

$$f(x) = \sum_{S \subset [n]} \widehat{f}(S)\, \chi_S(x), \tag{13}$$

called the *Fourier expansion*, with *Fourier coefficients* given by the inner products with the parity functions

$$\widehat{f}(S) = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x)\chi_S(x) = \langle f, \chi_S \rangle. \tag{14}$$

We refer to the mapping from $f(x)$ to $\widehat{f}(S)$ as the *Fourier transform* of f. The sparsity of f, denoted $\text{spar}(f)$, is the number of non-zero coefficients $\widehat{f}(S)$. When $\text{spar}(f) = \text{poly}(n)$ we refer to f as *polynomially sparse*. f,

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[2]Projectors also give quantum observables. In particular, for an arbitrary normalized n-qubit state $|\psi\rangle$, the probability p_1 of a computational basis measurement returning a satisfying string (i.e., an x such that $f(x) = 1$) is given by $p_1 = \langle\psi|H_f|\psi\rangle$, i.e., is equal to the expected value of repeated measurements of H_f on the state $|\psi\rangle$.

denoted $\deg(f)$, is defined to be the largest $|S|$ such that $\widehat{f}(S)$ is nonzero. Note that if f depends on only $k \leq n$ variables, then $\deg(f) \leq k$.

Hence, using the Fourier expansion and the identification $\chi_S \simeq Z_S = \bigotimes_{j \in S} Z_j = \prod_{j \in S} Z_j$ as explained above, an arbitrary Boolean function f is represented as a linear combination of tensor products of Z_j operators. Recall that we define the degree of such a Hamiltonian H_f, $\deg(H_f)$, to be the largest number of qubits acted on by any term in this sum, and the size of H_f, $\text{size}(H_f)$, to be the number of (nonzero) terms. Clearly, we have $\deg(H_f) = \deg(f)$ and $\text{size}(H_f) = \text{spar}(f)$. In particular, polynomially sparse functions yield Hamiltonians of size $\text{poly}(n)$.

Observe that, as all Pauli operators and their tensor products are traceless except for the identity operator, we have $\widehat{f}(S) = \text{tr}(H_f \prod_{j \in S} Z_j)/2^n$ where $\text{tr}(H)$ denotes the *trace* of the matrix H, i.e., the sum of its diagonal elements, which in particular is a basis-independent linear function [20]. Moreover, as the Pauli operators and their tensor products satisfy $\sigma_a \sigma_b = I$ if and only $\sigma_a = \sigma_b$, we further have $\widehat{f}(S) = \langle + |^{\otimes n} H_f \prod_{j \in S} Z_j |+\rangle^{\otimes n}$, i.e., each $\widehat{f}(S)$ also gives the expected value of the observable $H_f \prod_{j \in S} Z_j$ when measured on the equal super-position state $|+\rangle^{\otimes n}$.

We summarize our results on the representation of Boolean functions in the following theorem, which generalizes Proposition 1 above.

Theorem 2. *For an n-bit Boolean function $f \in \mathcal{B}_n$ of degree $d = \deg(f)$ the unique n-qubit Hamiltonian satisfying $H_f |x\rangle = f(x)|x\rangle$ in the computational basis is*

$$H_f = \sum_{S \subset [n], |S| \leq d} \widehat{f}(S) \prod_{j \in S} Z_j$$

with $\deg(H_f) = d$ and $\text{size}(H_f) \leq (e/d)^{d-1} n^d + 1$.

The coefficients $\widehat{f}(S)$ are defined as

$$\widehat{f}(S) = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x)(-1)^{S \cdot x} = \frac{1}{2^n} \text{tr}(H_f \prod_{j \in S} Z_j),$$

with $\widehat{f}(\emptyset) \in [0,1]$, and $\widehat{f}(S) \in [-\frac{1}{2}, \frac{1}{2}]$ for $S \neq \emptyset$, and satisfy

$$\sum_{S \subset [n]} \widehat{f}(S)^2 = \widehat{f}(\emptyset) = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x) = \frac{1}{2^n} \text{tr}(H_f) \tag{15}$$

Moreover,

$$\sum_{S \subset [n]} \widehat{f}(S) = f(0^n), \tag{16}$$

where 0^n denotes the input string of all 0s.

The results (15) and (16) are straightforward to derive by applying standard Fourier analysis such as Parseval's identity and using $f^2 = f$. The Hamiltonian size upper bound $\text{size}(H_f) \leq (e/d)^{d-1} n^d + 1$ follows from the binomial coefficient bound $\binom{n}{d} \leq n^d (e/d)^d / e$ for $d \geq 1$. Hence, if H_f acts on a constant number $d = O(1)$ of qubits, then its size is polynomially bounded in the number of qubits, $\text{size}(H_f) = O(n^d)$. Recall that we consider a family of n-bit functions f_n to be *efficiently representable* as the Hamiltonians H_{f_n} if $\text{size}(H_{f_n}) = \text{poly}(n)$ and the cost of computing each of the nonzero Fourier coefficients is also polynomially bounded with respect to n. Note that this notion of efficiency is only meaningful if f is given in a compact form, i.e., described by $\text{poly}(n)$ input bits to begin with.

We emphasize that the Hamiltonian coefficients $\widehat{f}(S)$ depend only on the function values $f(x)$, and are independent of *how* such a function may be represented as input (e.g., formula, circuit, truth table, etc.). Many typical compact representations of Boolean functions as computational input such as Boolean formulas (e.g. CNF, DNF, etc.) or Boolean circuits can be directly transformed to Hamiltonians using the composition rules of Theorem 1 which we derive below.

On the other hand, Theorem 2 shows that computing the Hamiltonian representation of Boolean functions is a computationally difficult problem in general. Consider a Boolean function f given as a formula in *conjunctive*

normal form, the AND of clauses containing ORs of variables and their negations. The satisfiability problem (SAT) is to decide if there exists a satisfying assignment for such an f. It is NP-hard to decide this for an arbitrary such function, even if clauses are restricted to at most 3 literals (3-SAT). Theorem 2 implies that computing the single Fourier coefficient $\widehat{f}(\emptyset)$ is equivalent to computing the *number* of satisfying assignments, which is believed to be a much harder problem. (In fact, this problem #SAT is complete for the counting complexity class #P; see e.g. [9].) Thus, the problem of deciding if $\widehat{f}(\emptyset) > 0$ is NP-hard, and computing $\widehat{f}(\emptyset)$ is #P-hard. This result is stated as Corollary 1 above. Moreover, arbitrary Boolean functions may have size exponential in n, in which case, even if we know somehow its Hamiltonian representation, we cannot implement or simulate this Hamiltonian efficiently (with respect to n) with the usual approaches.

As mentioned, Hamiltonians representing pseudo-Boolean functions, in particular, objective functions for constraint satisfaction problems, often avoid these difficulties. We are particularly interested in functions given as the sum of a number of *local* clauses C_j, where each clause acts on at most $k = O(1)$ bits (e.g., Max-k-Sat), and so the Hamiltonians H_{C_j} representing each clause have degree $O(1)$ and size $O(1)$, and hence can be efficiently constructed. Applying the well-known results of [13, Thm. 1 & 2] for such functions to Theorem 2 immediately gives the following useful result.

Proposition 5. *For a function $f \in \mathcal{B}_n$ that depends only on $k \leq n$ variables, represented as a Hamiltonian H_f acting on n qubits, the degree of H_f satisfies*

$$k \geq D(f) \geq \deg(H_f) \geq \log_2 k - O(\log \log k), \tag{17}$$

where $D(f)$ is the decision tree complexity of f and $D(f) = O(\mathrm{poly}(\deg(H_f)))$.

We remark that many other important properties of Boolean functions follow from their Fourier expansion, and other related results from the literature concerning the Fourier analysis of Boolean functions, such as, e.g., those of [16], may be similarly adapted to obtain further properties of corresponding Hamiltonians.

2.1.1 Composition Rules

Boolean functions arise in many different applications, but are often given in or easily reduced to a *normal form*. For example, SAT formulas are given in conjunctive normal form (CNF). Many other normal forms exist such as disjunctive (maxterms), algebraic ($\oplus$), etc. [21]. Note that while logically equivalent, the different forms may be very different for computational purposes. For each form there corresponds a notion of size (which directly relates to the number of bits needed to describe a function in such a form).

Therefore, it is especially useful to have a methodical way to combine Hamiltonians representing basic Boolean elements (functions) in order to construct representations of conjunctions (AND), disjunctions (OR), etc. of these elements. First consider Hamiltonians representing basic elements. The trivial functions $f = 0$ and $f = 1$ are represented by the Hamiltonians $H_0 = 0$ and $H_1 = I$, respectively. Using the identity $(-1)^x = 1 - 2x$, we represent the jth variable x_j, considered as a multiplication operator, as the Hamiltonian

$$H_{x_j} = I^{\otimes j-1} \otimes |x_j\rangle\langle x_j| \otimes I^{\otimes n-j} = \frac{1}{2}(I - Z_j),$$

which acts as $H_{x_j}|x\rangle = x_j|x\rangle$. Similarly, $H_{\overline{x}_j} = I/2 + Z_j/2$. For convenience, when no ambiguity arises, we will sometimes write x_j to mean the Hamiltonian H_{x_j}, and likewise for other basic functions. Similarly, for clarity we avoid writing tensor factors of identity operators explicitly when there is no ambiguity.

We summarize the Hamiltonian representations of several basic Boolean functions in Table 1 above, which are easily derived from Theorem 2. By applying the laws of propositional logic, we may derive analogous rules for composing Hamiltonians representing basic clauses to construct representations of clauses with arbitrary numbers of variables, clauses mixing arbitrary operations, or higher-order Boolean functions such as nested Boolean formulas and Boolean circuits. This approach often allows for easier construction of the Hamiltonian than by working with the Fourier expansion directly.

We summarize some important composition rules in Theorem 1 above. It is straightforward to extend Theorem 1 to other operations using the same technique of the proof.

Proof of Thm. 1. The logical values 1 and 0 (*true* and *false*) are represented as the identity matrix I and the zero matrix, respectively. Each result follows from the natural embedding of $f, g \in \mathcal{B}_n$ into $\mathcal{R}_n$, the

real vector space of real functions on n bits. From linearity of the Fourier transform, we immediately have $H_{af+bg} = aH_f + bH_g$ for $a, b \in \mathbb{R}$. Using standard identities, Boolean operations $(\cdot, \vee, \oplus, \dots)$ on f, g can be translated into $(\cdot, +)$ formulas, i.e., linear combinations of f and g. Linearity then gives the resulting Hamiltonian in terms of H_f and H_g. Explicitly, for the complement of a function $\overline{f}$, as $\overline{f} = 1 - f$, we have $H_{\overline{f}} = I - H_f$. Similarly, the identities $f \wedge g = fg$, $f \vee g = f + g - fg$, $f \oplus g = f + g - 2fg$, and $f \Rightarrow g = \overline{f} + fg$, respectively, imply the remainder of the theorem. $\qquad\square$

The rules of Theorem 1 may be applied *recursively* to construct Hamiltonians representing more complicated Boolean functions, corresponding e.g. to parentheses in logical formulas, or wires in Boolean circuits. For example, the Hamiltonian representing the Boolean clause $f \vee g \vee h = f \vee (g \vee h)$ is given by $H_{f \vee g \vee h} = H_f + H_{g \vee h} - H_f H_{g \vee h}$, which simplifies to $H_{f \vee g \vee h} = H_f + H_g + H_h - H_f H_g - H_f H_h - H_g H_h + H_f H_g H_h$.

Some typical examples of Boolean functions on 3 variables are the Majority (MAJ), Not-All-Equal (NAE), and 1-in-3 functions, which behave as their names indicate. The Mod_3 function is 1 when the sum $x_1 + x_2 + x_3$ is divisible by 3, and satisfies $\text{Mod}_3 = \overline{NAE}$. We show the Hamiltonians representing these functions in Table 2, which may be derived using the Fourier expansion results of Theorem 2 or the composition rules of Theorem 1. For example, H_{1in3} follows applying Thm. 1 with the identity $1in3(x_1, x_2, x_3) = x_1 \overline{x}_2 \overline{x}_3 + \overline{x}_1 x_2 \overline{x}_3 + \overline{x}_1 \overline{x}_2 x_3$.

$f(x)$	H_f
$MAJ(x_1, x_2, x_3)$	$\frac{1}{2}I - \frac{1}{4}(Z_1 + Z_2 + Z_3 - Z_1 Z_2 Z_3)$
$NAE(x_1, x_2, x_3)$	$\frac{3}{4}I - \frac{1}{4}(Z_1 Z_2 + Z_1 Z_3 + Z_2 Z_3)$
$MOD_3(x_1, x_2, x_3)$	$\frac{1}{4}I + \frac{1}{4}(Z_1 Z_2 + Z_2 Z_3 + Z_1 Z_3)$
$1in3(x_1, x_2, x_3)$	$\frac{1}{8}(3I + Z_1 + Z_2 + Z_3 - Z_1 Z_2 - Z_2 Z_3 - Z_1 Z_3 - 3Z_1 Z_2 Z_3)$

Table 2: Hamiltonians representing Boolean functions on three variables.

Together, the rules of Theorem 1 and Table 1 show how to construct Hamiltonians representing functions given as arbitrary Boolean algebra$(\wedge, \vee)$ or Boolean ring$(\cdot, \oplus)$ elements, which are complete in the sense of representing all possible Boolean functions [21].

2.2 Pseudo-Boolean Functions and Constraint Satisfaction Problems

Real functions on n-bits are similarly represented as Hamiltonians via the Fourier transform. Every such function $f \in \mathcal{R}_n$ may be expanded (non-uniquely) as a weighted sum of Boolean functions, possibly of exponential size. By linearity of the Fourier transform, the Hamiltonian H_f is given precisely by the corresponding weighted sum of the Hamiltonians representing the Boolean functions. Moreover, the Hamiltonian H_f is unique, so different expansions of f as sums of Boolean functions must all result in the same H_f.

The Fourier coefficients are again given by the inner product (12) with the parity functions χ_S,

$$\widehat{f}(S) = \langle f, \chi_S \rangle = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x) \chi_S(x), \tag{18}$$

and these coefficients again lead directly to the Hamiltonian H_f representing f. We are particularly interested in *pseudo-Boolean functions* given as a weighted sum of clauses

$$f(x) = \sum_{j=1}^{m} w_j f_j(x), \tag{19}$$

where $f_j \in \mathcal{B}_n$ and $w_j \in \mathbb{R}$. In a *constraint satisfaction problem*, typically all $w_j = 1$ and hence $f(x)$ gives the number of satisfied clauses (constraints). See [5,7] for Hamiltonian constructions for a variety of such problems.

We have the following result which extends the previous results for Boolean functions.

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Theorem 3. *An n-bit real function $f : \{0,1\}^n \to \mathbb{R}$ is represented as the Hamiltonian*

$$H_f = \sum_{S \subset [n]} \widehat{f}(S) \prod_{j \in S} Z_j, \qquad \widehat{f}(S) = \langle f, \chi_s \rangle = \mathrm{tr}(H_f \prod_{j \in S} Z_j) \in \mathbb{R}.$$

In particular, a pseudo-Boolean function $f = \sum_{j=1}^m w_j f_j$, $w_j \in \mathbb{R}$, $c_j \in \mathcal{B}_n$, is represented as

$$H_f = \sum_{j=1}^m w_j H_{f_j},$$

with $\deg(H_f) = \max_j \deg(f_j)$ and $\mathrm{size}(H_f) \leq \min\{\sum_j \mathrm{size}(H_{f_j}), (e/d)^{d-1} n^d + 1\}$.

The theorem follows from Theorem 2 and the linearity of the Fourier expansion, and implies Proposition 2 given previously. Thus the results of Theorems 1 and 2 for Boolean functions also apply to the construction of Hamiltonians representing real functions.

Remark 1. *In contrast to Theorem 2, for a constraint satisfaction problem $f = \sum_{j=1}^m f_j$, $f_j \in \mathcal{B}_n$, applying Parseval's identity we have*

$$\sum_{S \subset [n]} \widehat{f}(S)^2 = \mathbf{E}[f] + 2 \sum_{i<j} \langle f_i, f_j \rangle = \widehat{f}(\emptyset) + 2 \sum_{i<j} \mathbf{E}[f_i \wedge f_j] \geq \mathbf{E}[f],$$

where $\mathbf{E}[f] := \frac{1}{2^n} \sum_{x \in \{0,1\}^n} f(x)$ gives the expected value of $f(x)$ over the uniform distribution. In particular, $\sum_{S \subset [n]} \widehat{f}(S)^2 = \mathbf{E}[f]$ if and only if $\langle f_i, f_j \rangle = 0$ for all i, j. If there does exist an i, j such that $\langle f_i, f_j \rangle = 0$, then the conjunction of the clauses is unsatisfiable, i.e. $\wedge_j f_j = 0$.

2.2.1 Simulating Diagonal Hamiltonians

In many applications we are required to *simulate* a Hamiltonian H for some time parameter $\gamma \in \mathbb{R}$, i.e., implement exactly or approximately the unitary operator

$$U(\gamma) = e^{-i\gamma H}.$$

Consider the simulation of a Hamiltonian H_f representing a real or Boolean function f. It is well known that if f can be efficiently computed classically, and if ancilla qubits are available, then the Hamiltonian H_f can be simulated efficiently by computing f in a register and performing a sequence of controlled rotations; see, e.g., [22]. These methods typically avoid computing H_f explicitly. On the other hand, there exist applications where an explicit Hamiltonian-based implementation is desirable, such as quantum annealing, or cases where we wish to minimize the need for ancilla qubits, such as, for example, near-term or low-resource applications.
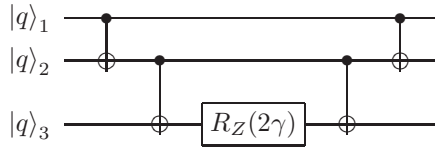

Fig. 1: Quantum circuit performing the operation $U = exp(-i\gamma Z_1 Z_2 Z_3)$ on three qubits labeled 1, 2, and 3. The middle operator is a Z-rotation gate, and the other gates are controlled-NOT (CNOT) gates with a black circle indicating the control qubit and cross indicating the target. By similar circuits, $U = exp(-i\gamma Z_1 Z_2 \ldots Z_\ell)$ can be implemented with $2(\ell - 1)$ CNOT gates and one R_Z gate. Different circuit compilations are possible, including compilation to different gate sets.

Efficient circuits simulating products of Pauli Z operators are well-known [22,23], as shown in Figure 1. As Pauli Z terms mutually commute, circuits for individual terms in the Hamiltonians (2) or (4) can be applied in sequence to simulate their sum. Thus, for a given Hamiltonian H_f representing a general Boolean or pseudo-Boolean function, if $\mathrm{size}(H_f) = O(\mathrm{poly}(n))$, then we can simulate H_f efficiently. Applying these circuits to our previous results, we have the following corollary.

Corollary 2. *A Hamiltonian H_f representing a Boolean or real function as in (2) or (4) can be simulated, i.e., the operation $exp(-i\gamma H_f)$ implemented for $\gamma = O(1)$, with n qubits and $O(\deg(H_f) \cdot size(H_f))$ basic quantum gates. In particular, Hamiltonians H_f with bounded maximum degree $\deg(H_f) = d = O(1)$ can be simulated with $O(n^d)$ basic gates. Ancilla qubits are not necessary in either case.*

Here, by *basic quantum gates* we mean the set of CNOT and single qubit rotation gates, which is a standard universal set [17, 23]. We remark that the Hamiltonian simulation considered in the corollary is exact in the sense that if each of the basic gates is implemented exactly, then so is $exp(-i\gamma H_f)$. The approximation of quantum gates and operators is an important topic but we do not deal with it here; see, e.g., [17].

Remark 2. *For a Hamiltonian H_f representing a Boolean function f, simulating H_f for time π gives the oracle query for Grover's algorithm [17]*

$$e^{-i\pi H_f}|x\rangle = (-1)^{f(x)}|x\rangle. \tag{20}$$

Hence, when H_f is known explicitly and $size(H_f) = \text{poly}(n)$, we can efficiently construct and implement the operator $(-1)^{f(x)}$ using quantum circuits for simulating H_f, which can be compiled to CNOT and R_Z gates. We elaborate on the relationships between different types of queries for accessing a function as input to a quantum algorithm in Appendix A.4.

2.2.2 Quadratic Unconstrained Binary Optimization

A general and important class of pseudo-Boolean optimization problems are *quadratic unconstrained binary optimization* (QUBO) problems [3], where we seek to maximize or minimize a degree two function

$$f(x) = a + \sum_{j=1}^{n} c_j x_j + \sum_{j<k} d_{jk} x_j x_k, \tag{21}$$

with $a, c_j, d_{jk} \in \mathbb{R}$, $x_j \in \{0, 1\}$. Indeed, this is the class of problems (ideally) implementable on current quantum annealing devices such as, for example, D-WAVE machines, where the qubit interactions are themselves quadratic [3, 24]. The QUBO class also contains many problems which at first sight are not quadratic, via polynomial reductions which often require extra variables; indeed, the natural QUBO decision problem is NP-complete [25]. Note that $\overline{x}_j = 1 - x_j$, so (21) is without loss of generality.

Proposition 6. *The QUBO function (21) maps to a Hamiltonian given as a quadratic sum of Pauli Z operators, with $size(H_f) \leq 1 + n/2 + n^2/2$. Explicitly, we have*

$$H_f = (a + c + d)I - \frac{1}{2}\sum_{j=1}^{n}(c_j + d_j)Z_j + \frac{1}{4}\sum_{j<k} d_{jk} Z_j Z_k, \tag{22}$$

where we have defined $c = \frac{1}{2}\sum_{j=1}^{n} c_j, d = \frac{1}{4}\sum_{j<k} d_{jk}$, and $d_j = \frac{1}{2}\sum_{k:k\neq j} d_{jk}$ with $d_{jk} = d_{kj}$.

Moreover, we can simulate H_f, i.e., implement the phase operator $U_p(t) = e^{-itH_f}$, using at most n many R_Z rotation gates and $\binom{n}{2}$ many R_{ZZ} gates.

Proof. Applying Theorems 1 and 3 to (21) gives (22). As the terms in (22) mutually commute, each term can be simuated individually, which gives the cost estimates in terms of Pauli rotation gates. Note that each R_{ZZ} can be simulated with two CNOT gates and a R_Z gate, see Figure 1 above. $\square$

The QUBO problem is closely related to the Ising model of interacting spins from physics, and to various related models describing the behavior of *spin glasses* [26].

Remark 3 (Interacting spin systems). *Consider the ISING decision problem of determining whether the ground state energy (lowest eigenvalue) of an Ising model (degree two) diagonal Hamiltonian*

$$H = a_0 I + \sum_j a_j Z_j + \sum_{j<k} a_{jk} Z_j Z_k$$

is at most a given constant. As the number of terms is $size(H) = O(n^2)$, we can efficiently check the energy of a candidate ground state, so the problem is in NP. On the other hand, from Theorem 1, we have that the

NP-complete problem MAX-2-SAT maps to a degree-two Hamiltonian of this form, with solution corresponding to the ground state energy of $-H$. Thus, from our results it trivially follows that ISING is NP-complete. Similar arguments can be used to show NP-completeness with restricted values of the coefficients (e.g., antiferromagnetic) or with restricted interaction graphs such as planar (two-dimensional) graphs [27].

3 Non-diagonal Hamiltonians and Unitaries

The results of Theorem 3 show that the 2^n-dimensional space of diagonal Hamiltonians, i.e., Hamiltonians given as linear combinations of Pauli Z operators, is isomorphic to the vector space of real functions on n bits. Similarly, the tensor products of Pauli matrices give a basis for the vector space of n-qubit Hamiltonians. Hence, a general Hamiltonian H may be expanded as a linear sum

$$H = a_0 I + \sum_{j=1}^{n} \sum_{\sigma=X,Y,Z} a_{j\sigma}\sigma_j + \sum_{j\neq k} \sum_{\sigma=X,Y,Z} \sum_{\lambda=X,Y,Z} a_{jk\sigma\lambda}\sigma_j\lambda_k + \dots, \tag{23}$$

with $a_\alpha \in \mathbb{R}$. Thus, an arbitrary Hamiltonian on n qubits is uniquely specified by 4^n real coefficients. Unlike the Hamiltonians (2) and (4) representing Boolooean and real functions, the terms in H do not mutually commute in general, and H can act non-diagonally and with complex amplitude on computational basis states.

Using the properties of the Pauli matrices and applying arguments similar to those of Section 2, the coefficients of the Hamiltonian (23) are easily shown to satisfy

$$a_\alpha = \frac{1}{2^n}\text{tr}(\alpha H), \tag{24}$$

for each of the 4^n Pauli terms $\alpha = \sigma_1\sigma_2\dots\sigma_n$, $\sigma_j \in \{I, X_j, Y_j, Z_j\}$.

We leave the detailed consideration of general Hamiltonians and unitaries to future work. In the remainder of this section, we show how our results for diagonal Hamiltonians may be used to construct and analyze useful classes of non-diagonal Hamiltonians such as controlled operations and operators computing functions in ancilla qubit registers.

3.1 Controlled Unitaries

In many applications we require controlled Hamiltonian evolutions. For example, in quantum phase estimation (QPE) [17], we require transformations on $(1+n)$-qubit basis states of the form

$$|0\rangle|x\rangle \to |0\rangle|x\rangle, \qquad |1\rangle|x\rangle \to e^{-iHt}|1\rangle|x\rangle,$$

for various values $t = 1, 2, 4, \dots$. Consider such a transformation with fixed t. Labeling the first register (control qubit) a, the overall unitary may be written as

$$\Lambda_{x_a}(e^{-iHt}) = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes e^{-iHt}. \tag{25}$$

Recall the notation $\Lambda_{x_a}(e^{-iHt})$ indicates the unitary e^{-iHt} controlled by the classical function x_a. We obtain the Hamiltonian corresponding to this transformation by writing $\Lambda_{x_a}(e^{-iHt}) = e^{-i\widetilde{H}t}$, which gives

$$\widetilde{H} = |1\rangle\langle 1| \otimes H = x_a \otimes H = \frac{1}{2}I \otimes H - \frac{1}{2}Z_a \otimes H. \tag{26}$$

Recall that for simplicity we sometimes write a function f in place of its Hamiltonian representation H_f as we have done here for the function $f(x) = x_a$. Note that the control qubit is assumed precomputed here; its value may or may not depend on x.

More generally, consider Hamiltonian evolution controlled by a Boolean function $g \in \mathcal{B}_k$ acting on a k-qubit ancilla register. In this case we seek to affect the unitary transformation on $(k+n)$-qubit basis states

$$|y\rangle|x\rangle \to |y\rangle|x\rangle \qquad \text{if } g(y) = 0,$$

$$|y\rangle|x\rangle \to e^{-iHt}|y\rangle|x\rangle \qquad \text{if } g(y) = 1,$$

which gives the overall unitary

$$\Lambda_g(e^{-iHt}) = \sum_{y:g(y)=0} |y\rangle\langle y| \otimes I + \sum_{y:g(y)=1} |y\rangle\langle y| \otimes e^{-iHt} = H_{\overline{g}} \otimes I + H_g \otimes e^{-iHt}, \tag{27}$$

corresponding to evolution under the Hamiltonian

$$\widetilde{H}_g = \sum_{y:g(y)=1} |y\rangle\langle y| \otimes H = H_g \otimes H. \tag{28}$$

These results have been summarized in Proposition 3 above.

Remark 4. *Consider a bit-flip operation controlled by the bit itself. This is represented by the Hamiltonian Xx which acts as $Xx|0\rangle = 0$ and $Xx|1\rangle = |0\rangle$. However, we have $Xx = X(I - Z)/2 = X/2 + iY/2$, which is not self-adjoint. Thus, applying equation (27) to the case where H_g and H act on overlapping qubits is not guaranteed to produce self-adjoint operators, i.e., the resulting $\widetilde{H}_g$ may not give a Hamiltonian.*

Indeed, the operator Xx is equivalently the well-known spin annihilation operator $b = |0\rangle\langle 1|$. The spin creation operator $b^\dagger$ is similarly given as $b^\dagger = (Xx)^\dagger = xX = X\overline{x}$, and the spin number (occupation) operator is $b^\dagger b = x = (I - Z)/2$.

Note that if the Hamiltonian $H = H_f$ represents a Boolean function f, then (28) represents the conjunction of f and g, i.e., we have $\widetilde{H}_g = H_g \otimes H_f = H_{g \wedge f}$.

Moreover, for an arbitrary Hamiltonian H, if we can implement the ancilla controlled operator $\Lambda_{x_a}(e^{-iHt})$ for sufficiently many values of $t \in \mathbb{R}$, then it is straightforward to implement a variable-time controlled Hamiltonian simulation operator Λ_H, which acts on computational basis states as

$$\Lambda_H |t\rangle|x\rangle = |t\rangle e^{-iHt}|x\rangle. \tag{29}$$

For example, if t was encoded in binary, then Λ_H could be implemented by applying the operators $\Lambda_{x_{a_0}}(U(2^0 t))$, $\Lambda_{x_{a_1}}(U(2^1 t))$, ..., $\Lambda_{x_{a_j}}(U(2^j t))$ in sequence controlled over each bit a_j in the first register; see, e.g., [17].

3.2   Computing functions in registers

Suppose for a Boolean function f we have a unitary operator G_f that acts on each $(n + 1)$-qubit basis state $|x\rangle|a\rangle$, $a \in \{0, 1\}$ as

$$G_f|x\rangle|a\rangle = |x\rangle|a \oplus f(x)\rangle. \tag{30}$$

If we let the function f be arbitrary and unknown, then each application of G_f (considered a black-box) is called an *oracle query* for f. Operators G_f as in (30) are called *bit queries*. Note that G_f may often be derived from a reversible classical circuit for computing f, but we consider it abstractly here. (In contrast, the query for Grover's algorithm given in (20) is often referred to as a *phase query*.)

Observe that the (non-diagonal) Hamiltonian

$$H'_f := G_f x_a G_f = \frac{1}{2}I - \frac{1}{2}G_f Z_a G_f$$

acts on computational basis states as

$$H'_f|x\rangle|a\rangle = f(x)|x\rangle|a\rangle, \tag{31}$$

so in this sense H'_f also gives a representation of f.

In Proposition 4 above, we show that computing a Boolean function in a register is closely related to computing it as an amplitude.

Proof of Prop. 4. Using Prop. 3 with H_f as given in Thm. 2 and $H = X_a$, we expand G_f as a sum of Pauli matrices $G_f = (1 - \widehat{f}(\emptyset))I + \widehat{f}(\emptyset)X_a + \ldots$, where none of the terms to the right are proportional to I. Thus computing the identity coefficient of G_f gives (one minus) the number of satisfying assignments for f. □

4   Discussion

We have derived explicit rules and results for constructing Hamiltonians representing Boolean and pseudo-Boolean functions, and in particular objective functions for constraint satisfaction problems. Moreover, we have shown how to construct controlled unitaries at the level of Hamiltonians. The goal of these results is to give a toolkit which can be used generally for designing and implementing quantum algorithms for approximate optimization and related applications such as machine learning [28], in both the quantum gate model and in quantum annealing. Our results give a unified approach to understanding existing problem mappings in the literature, such as those of [5, 7].

There are several enticing applications and extensions of our results, and we briefly describe several in the appendix. We emphasize that Fourier analysis is generally a very rich topic in computer science, mathematics, and physics, in addition to its many applications in quantum computing. A promising research direction is to further apply these tools, in particular the Fourier analysis of Boolean functions as applied in classical computing, to the design and analysis of quantum algorithms. As mentioned, we leave a detailed analysis of fully general (non-diagonal) Hamiltonians as a topic of future work. A next step is to further study *unfaithful* representations of Boolean functions, where n variables are encoded in some number $n' > n$ of qubits, which in particular is an important paradigm for embedding problems on physical quantum annealing hardware, and, more generally, is related to the theory of quantum error correcting codes [17]. Moreover, our results may have useful applications to physics, where many important Hamiltonians are given as linear combination of Pauli operators, such as the Ising or quantum XY models [27, 29]. Furthermore, applications to quantum complexity theory may also be of interest, such as the complexity of local Hamiltonian eigenvalue problems [30], Hamiltonian complexity [31, 32], and the computational power of instantaneous quantum polynomial-time [33] or low-depth [28, 34] quantum circuits.

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A   Some Applications

As explained, representing functions as Hamiltonians is a critical component of mapping optimization problems to quantum algorithms such as quantum annealing or QAOA.

In this section we outline several other applications of our results.

A.1   Penalty terms for constrained optimization

In constrained optimization problems, we seek an optimal solution subject to satisfying a set of *feasibility* constraints. These constraints may arise as part of the problem itself or from its encoding; see [5, 7] for examples. In quantum annealing, a common approach to dealing with problem constraints is to augment the Hamiltonian that represents the objective function to be minimized with additional diagonal Hamiltonian terms that penalize (i.e., shift the eigenvalues of) states outside of the feasible subspace [3, 7].

For example, suppose we are given a real function $f(x)$ to minimize, and a set of Boolean constraint functions g_j, $j = 1, \ldots, \ell$, such that $g_j(x) = 1$ implies x is an infeasible state, and $\sum_j g_j(x) = 0$ if and only if x is feasible. We may construct the augmented problem Hamiltonian as

$$H_p = H_f + \sum_{j=1}^{\ell} w_j H_{g_j},$$

where the Hamiltonians H_f and H_{g_j} represent f and the g_j as in Theorems 3 and 2, respectively. The w_j are positive weights which may be selected appropriately such that infeasible states are eigenvectors of H_p with

eigenvalues greater than $\|H_f\|$, and feasible states are eigenvectors with eigenvalues $f(x)$. Hence, the ground state subspace of H_p is spanned by states representing optimal feasible problem solutions.

Thus, Theorems 1, 2, and 3 may be used to explicitly construct problem mappings with penalty terms.

A.2 Ground state Boolean logic

With a universal quantum computer, a single control bit suffices for all efficiently computable control functions [17]. Indeed, we can always compute a Boolean function $f(x)$ in a register by constructing a unitary operator $U_f : |x\rangle|a\rangle \to |x\rangle|a \oplus f(x)\rangle$ as we considered in Section 3.2. Nevertheless, in certain applications it is desirable to have a purely Hamiltonian implementation; for example, in a restricted computational model such as that of the DWAVE quantum annealers, which is generally not believed to be universal for quantum computation.

One approach to computing a Boolean function $f \in \mathcal{B}_f$ in a register is to encode its input-output pairs as the ground state subspace of a Hamiltonian H, referred to as ground state Boolean logic; see, e.g., [35–37]. For example, the function $AND(x, y) = xy$ can be encoded as the subspace $span\{|x\rangle|y\rangle|xy\rangle\} = span\{|000\rangle, |010\rangle, |100\rangle, |111\rangle\}$.

There are many different ways to encode such a function as the ground state subspace of a Hamiltonian, as there is freedom in how exactly the Hamiltonian acts on invalid computational basis states $|x\rangle|y\rangle|z\rangle$ with $z \neq xy$. The penalty term approach of the previous section could be used to penalize the invalid states. An alternative construction is to directly implement the Boolean function $g \in \mathcal{B}_{n+1}$ satisfying $g(x, y) = 0$ if and only if $y = f(x)$, which equivalently is given by $g(x, y) = \overline{f(x) \oplus y}$. Applying Theorems 1 and 2 to this function and simplifying gives the following result.

Proposition 7. *Let $f \in \mathcal{B}_n$ be represented by the Hamiltonian H_f as in Theorem 2. Then the $(n + 1)$-qubit Hamiltonian H_g*

$$H_g = I \otimes x_a + H_f \otimes Z_a \tag{32}$$

has ground state subspace given by

$$span\{|x\rangle|f(x)\rangle : x \in \{0, 1\}^n\},$$

and, in particular, H_g represents the Boolean function $g \in \mathcal{B}_{n+1}$ which satisfies $g(x, y) = 0$ if and only if $y = f(x)$.

Simpler Hamiltonians with the same ground state subspace may be found for specific classes of Boolean functions f; see, e.g., [24]. An advantage of the construction (32) is that it applies generally.

A.3 Approximate Hamiltonians

There are several proposed methods for reducing implementation costs related to a given Hamiltonian. Techniques for reducing Hamiltonian locality in the setting of quantum annealing such as perturbative gadgets are proposed in [35, 38, 39]; fortunately, arbitrary order interactions may be reduced, with some cost, to Hamiltonians with at most 2-local (quadratic) interactions [35], which are experimentally favorable [17].

In some applications it may be possible to reduce the implementation cost of a given Hamiltonian by instead using an approximate Hamiltonian. For example, using a Hamiltonian which approximately represents a given objective function for the phase operator in QAOA may significantly reduce the required circuit depth and size. Similar considerations apply to quantum annealing applications, and may be useful towards increasing the sizes of problems embeddable on current hardware. A further potential application is to perform a quantum anneal using an approximate Hamiltonian as a means of initial state preparation within a larger quantum algorithm. Generally, it remains an open problem to quantify the effect of such approximations on the performance of quantum algorithms such as quantum annealing or QAOA. Here, we briefly consider diagonal Hamiltonians representing approximations of Boolean functions. Similar ideas apply to approximations using, and of, non-diagonal Hamiltonians.

A function $\widetilde{f} \in \mathcal{R}_n$ *approximates* $f \in \mathcal{B}_n$ in the max norm [13] if

$$\forall x \in \{0, 1\}^n \quad |\widetilde{f}(x) - f(x)| \leq \frac{1}{3}. \tag{33}$$

The approximate degree of f, $\widetilde{\deg}(f)$, is defined to be the the minimal degree of Fourier polynomials $\widetilde{f}$ of the form (13) that approximate f. For example, $\widetilde{\deg}(OR_n) = O(\sqrt{n})$ [13] whereas $\deg(OR_n) = n$. We likewise

say a (diagonal) Hamiltonian $\widetilde{H}_f$ approximates a Hamiltonian H_f representing a Boolean function f if

$$\|\widetilde{H}_f - H_f\| \leq \frac{1}{3},$$

where clearly $\deg(\widetilde{H}_f) \geq \widetilde{deg}(f)$. Note that for diagonal matrices H, most matrix norms are equivalent, in particular $\|H\|_2 = \|H\|_1 = \|H\|_\infty$.

For example, on 2 qubits $AND = \frac{1}{4}(I - Z_1 - Z_2 + Z_1 Z_2)$ is approximated by $\widetilde{AND} = \frac{1}{3} - \frac{1}{6}Z_1 - \frac{1}{6}Z_2$, and OR is approximated by $\widetilde{OR} = \frac{1}{3} - \frac{1}{6}Z_1 - \frac{1}{6}Z_2$. Both of these approximations reduce the Hamiltonian degree by one. On the other hand, it is easy to show that no Hamiltonian of the form $aI + bZ_1 + cZ_2$ can approximate $x_1 \oplus x_2$. So this approach may have limited utility, or possibly it may only be useful for certain functions.

A.4 Phase kickback and query complexity

We use our results to illuminate the relationships between quantum circuits that compute a Boolean function f as a phase $e^{-itf(x)}$, and those that compute f in a register $|x\rangle|f(x)\rangle$, which are referred to as *phase queries* and *bit queries*, respectively. In particular, we show which oracles can efficiently simulate which others.

Let the Hamiltonian H_f represent f as in Theorem 2. Using an ancilla qubit initialized to $|0\rangle$, we can simulate H_f for time t, i.e., implement the operator $e^{-iH_f t}$, using two applications of the bit query G_f given in (30) and a Z-rotation gate R_Z applied to the ancilla register $|0\rangle_a$ as

$$e^{-iH_f t}|x\rangle|0\rangle = c \, G_f \, R_{Z_a}(-t) \, G_f |x\rangle|0\rangle, \tag{34}$$

where $c = e^{-it/2}$ is an irrelevant global phase. In particular, when $t = \pi$ we have $e^{-i\pi H_f} = (-1)^{f(x)}$, i.e., the Grover phase query (20), and a single application of G_f suffices

$$(-1)^{f(x)}|x\rangle|-\rangle = G_f|x\rangle|-\rangle$$

if we prepare the ancilla qubit state $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. This *phase kickback* is an important and well-known technique in quantum computation.

Conversely, if we can simulate H_f controlled by an ancilla qubit, i.e. implement the operator $\Lambda_{x_a}(e^{-i\pi H_f})$, then we can implement G_f using a single-bit *quantum phase estimation*, which requires two Hadamard gates and a controlled simulation of H_f. We have

$$G_f|x\rangle|0\rangle = \mathrm{H}_a \, \Lambda_{x_a}(e^{-i\pi H_f}) \, \mathrm{H}_a|x\rangle|0\rangle, \tag{35}$$

where H_a denotes the Hadamard gate [17] acting on the ancilla qubit a. Similarly, we can simulate $\Lambda_{x_a}(e^{-i\pi H_f})$ using an additional ancilla qubit $|0\rangle_b$ to store $f(x)$ as

$$\Lambda_{x_a}(e^{-itH_f})|a\rangle_a|x\rangle|0\rangle_b = (I \otimes G_f) \, \Lambda_{x_a x_b}(R_Z(-t)) \, (I \otimes G_f) \, |a\rangle_a|x\rangle|0\rangle_b, \tag{36}$$

where the doubly-controlled Z-rotation gate $\Lambda_{x_c x_a}(R_Z(-t))$ can be easily implemented using basic quantum gates [23]. Hence, in this sense the operations G_f and $\Lambda_{x_a}(e^{-itH_f})$ (for arbitrary t) are computationally equivalent. We refer to the operator $\Lambda_{x_a}(e^{-itH_f})$ as a *controlled phase query*.

Finally, observe that we can apply the construction (35) for G_f to (36) to yield

$$\Lambda_{x_a}(e^{-itH_f})|a\rangle_a|x\rangle|0\rangle_b = \mathrm{H}_b \, \Lambda_{x_b}(e^{-i\pi H_f}) \, \mathrm{H}_a \, \Lambda_{x_a x_b}(R_Z(-t)) \, \mathrm{H}_b \, \Lambda_{x_b}(e^{-i\pi H_f}) \, \mathrm{H}_b \, |a\rangle_a|x\rangle|0\rangle_b, \tag{37}$$

i.e., the query $\Lambda_{x_a}(e^{-itH_f}) = \Lambda_{x_a}((-1)^f)$ suffices to simulate $\Lambda_{x_a}(e^{-itH_f})$. As $\Lambda_{x_a}((-1)^{f(x)})$ also suffices to simulate G_f from (35), the oracles G_f, $\Lambda_{x_a}(e^{-itH_f})$, and $\Lambda_{x_a}((-1)^{f(x)})$ are computationally equivalent.

Thus, we obtain insight into the relative power of quantum circuits with bit query or phase query oracles. Define the computational reduction for quantum circuits A and B each acting on n qubits as $A \leq_q B$ if A can be simulated using at most $\mathrm{poly}(n)$ many calls to B, ancilla qubits, and quantum gates from a universal set. This relation is a preorder, and hence we may informally summarize the relations between theses oracles as

$$(-1)^{f(x)} \quad \leq_q \quad e^{-itf(x)} \, (t \in \mathbb{R}) \quad \leq_q \quad G_f \quad =_q \quad \Lambda_{x_a}((-1)^{f(x)}) \quad =_q \quad \Lambda_{x_a}(e^{-i\pi H_f}). \tag{38}$$

The relation (38) has immediate applications to quantum query complexity, i.e., the number of queries required for any quantum circuit computing a Boolean function. In particular, it implies that query lower

bounds obtained for bit queries, such as those of [14, 40], immediately give lower bounds to quantum circuits computing the same function using instead the phase or controlled-phase queries. Similarly, query complexity upper bounds for the phase oracles immediately give query upper bounds for the bit query or controlled phase query oracles.

We remark that the two inequalities in (38) can be shown to be strict, i.e., phase queries without control cannot efficiently simulate bit queries [41].

A.5 Fermionic Hamiltonians

For systems of fermions in the occupation number (second quantized) representation [42], Hamiltonians consist of linear combinations of fermionic creation and annihilation operators $a^\dagger$ and a. These operators satisfy the *canonical anticommutation relation* algebra

$$\{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0 \qquad \{a_j, a_k^\dagger\} = \delta_{jk}. \tag{39}$$

Recall the spin creation and annihilation operators $b^\dagger = (X - iY)/2$ and $b = (X + iY)/2$ of Remark 4, which satisfy a different algebra. It is easy to show that if we represent the fermionic operators using spin operators and the parity function χ_S, $S \subset [n]$ as

$$a_j = \chi_{\{1,2,\ldots,j-1\}} b_j \qquad a_j^\dagger = \chi_{\{1,2,\ldots,j-1\}} b_j^\dagger,$$

then the CAR relations (39) will be satisfied. Hence, from our previous results, we may represent these operators as

$$a_j = Z_1 Z_2 \ldots Z_{j-1}(X_j + iY_j)/2 \tag{40}$$

$$a_j^\dagger = Z_1 Z_2 \ldots Z_{j-1}(X_j - iY_j)/2, \tag{41}$$

which reproduces the well-known *Jordan-Wigner transform*. This representation is used in many applications, such as quantum algorithms for quantum chemistry.

We remark that it is straightforward to extend this result to implementing operators corresponding to Bogoliubov-transformed fermionic creation and annihilation operators $c_j^\dagger$ and c_j, which correspond to particular linear combinations of $a_j^\dagger$ and a_j; see, e.g., [29, 43]. An interesting direction of future research is to explore Hamiltonian representations of the various other operator algebras important in physics [43, 44].