Hamiltonian simulation with explicit formulas for digital-analog quantum computing

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Digital-analog is a quantum computational paradigm that employs the natural interaction Hamiltonian of a system as the entangling resource, combined with single qubit gates, to implement universal quantum operations. As in the case of its digital gate-based counterpart, designing digital-analog circuits that employ optimal quantum resources often requires an exceedingly large classical computational time. In this work we find a suboptimal solution to this exponentially large problem, showing that it can be solved within polynomial computational time. In particular, we provide an exact solution for the problem of expressing arbitrary two-body Hamiltonians as the sum of local unitary transformations of an arbitrary Ising Hamiltonian, with the total number of required terms being at most quadratic in system size. This allows us to design a digital-analog simulation protocol that avoids employing numerical optimization over a large parameter space at the preprocessing stage, minimizing computational resources and allowing for further scaling.

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I. INTRODUCTION

Universal quantum computation can be achieved through the application of different operations. In digital quantum computing one usually employs a universal set of discrete gates composed of arbitrary single qubit gates (SQGs) and two-qubit gates [1,2]. In contrast, digital-analog quantum computing (DAQC) employs the natural interaction Hamiltonian of a given system as the entangling resource [3]. By additionally implementing arbitrary SQGs on top of this evolution, we can implement any unitary operation [4]. This paradigm allows us to access the universality of the digital paradigm while benefiting from the noise resilience of analog quantum computations [5].

Although this set of operations is universal, composing the circuit that implements a particular operation employing the minimum resources is a highly nontrivial question [6–8]. When compiling a quantum circuit, minimizing the total number of gates employed and the total circuit time are essential computational efficiency factors [9]. In digital quantum computing, the total circuit time is dominated by the circuit depth and the total number of two-qubit gates, given that the application times of two-qubit gates are often slower than those of SQGs [10–13]. In DAQC, the total time is also dominated by the time where the system has been allowed to evolve freely under the natural Hamiltonian of the system, where all entangling operations are encoded [14,15].

In both paradigms, finding the optimal circuit is considered to be an NP-hard problem [16–18], and thus it is expected to consume exponentially many computing resources. As we do not expect this task to be efficiently solvable, one usually resorts to algorithms that take reduced time to find a suboptimal solution. While these protocols are usually available for the digital paradigm [19–21], they remain outstanding for digital-analog. The available methods to date require exponential resources to synthesize an optimal DAQC circuit for solving problems involving arbitrary Hamiltonians [17,22]. Solving these problems is fundamental not only for optimal generation of circuits in the DAQC paradigm, but also for the field of quantum simulation [23–25], where impressive experimental advances have been achieved in recent years [26–32]. Indeed, it is expected that DAQC will be able reproduce these milestones in quantum computing platforms, such as superconducting circuits [33,34], trapped ions [35,36], or neutral atoms [37,38], as these setups already provide all the capabilities required for the practical implementation of digital-analog circuits. Successfully simulating quantum systems might have direct applications in the fields of chemistry or condensed matter simulations among others [39–41].

In this work, we introduce a protocol for obtaining a suboptimal compilation in the simulation of arbitrary two-body Hamiltonians employing a DAQC circuit (see Fig. 1). Instead of restricting the protocol to single qubit gates from the Clifford group [16–18], here we employ arbitrary single qubit gates to design the circuit. The proposed protocol relies on the eigendecomposition a couplings matrix having size

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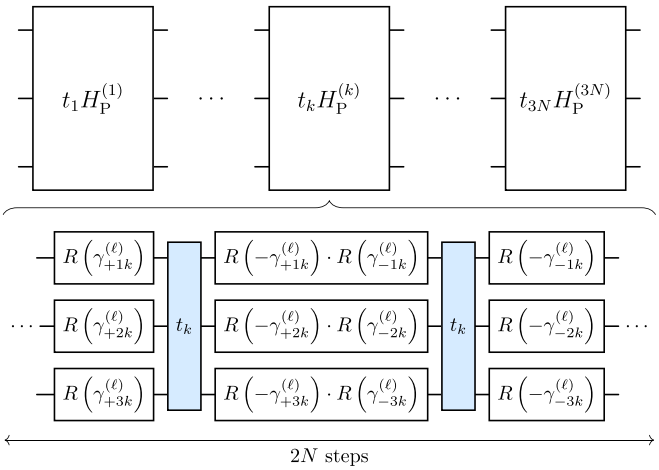

FIG. 1. Problem Hamiltonian decomposition and DAQC circuit sketch. The colored blocks correspond to analog blocks with evolution time t_k. The full circuit that simulates the evolution under the problem Hamiltonian for a time T, $TH_P = \sum_k t_k H_P^{(k)}$, is composed of up to $12N^2$ digital-analog blocks. The particular values of the rotation angles of the SQGs and t_k are given in Eq. (14).

$3N \times 3N$, with N being the number of qubits in the system. This allows us to produce a valid DAQC circuit with minimal computational resources, in particular in time $O(N^3)$. The protocol relies on closed-form formulas, thus removing the need to employ classical optimization algorithms to design the circuit. The resulting circuit is composed of at most $12N^2$ digital-analog blocks, resulting in a constant factor overhead over previous protocols, which required up to $9N(N-1)/2$ blocks. This way, we maintain the same asymptotic scaling as the state-of-the-art optimal protocols.

The rest of the paper is structured as follows. In Sec. II, we introduce the DAQC paradigm in detail and point out the main problem we are aiming to solve. Section III introduces the main result of the paper, providing a step-by-step description. In Sec. IV we report numerical calculations, comparing the output circuit times with previously known results. Finally, in Sec. V we discuss the results and provide some perspectives on the potential future applications of the protocol.

II. PRELIMINARIES ON DIGITAL-ANALOG QUANTUM COMPUTING

We can always describe a unitary operation in terms of the consecutive application of single qubit gates (SQGs) and evolution under entangling two-body Hamiltonians [4]. In DAQC these operations are implemented through the application of digital blocks, composed of SQGs, and analog blocks, in which the system freely evolves under the natural Hamiltonian of the system, the source Hamiltonian H_S [3]. However, connecting the unitary evolution of a desired problem Hamiltonian H_P and our resources is a nontrivial task in DAQC.

As a simple example, let us show how to simulate the evolution under a time-independent two-body ZZ Hamiltonian

$$H_P^{zz} = \sum_{i<j} h_{P_{ij}}^{zz} \sigma_i^z \sigma_j^z, \tag{1}$$

during a time T using as a resource another ZZ Hamiltonian

$$H_S = \sum_{i<j} h_{S_{ij}}^{zz} \sigma_i^z \sigma_j^z. \tag{2}$$

$\sigma_i^{\alpha=x,y,z}$ represent the standard Pauli matrices acting on qubit i, whereas $h_{P_{ij}}^{zz}$, $h_{S_{ij}}^{zz}$ represent the couplings in the problem and source Hamiltonians, respectively. This Hamiltonian is characteristic of trapped ions with Magnetic Gradient Induced Couplings (MAGIC) [36], among other systems. We employ a DAQC protocol in which the SGQs are restricted to be $X := \sigma^x$ gates [3]. This choice allows us to flip the effective sign of a coupling by conjugating it with an X gate in one of the two qubits, $\sigma_i^x e^{-iT\sigma_i^z\sigma_j^z}\sigma_i^x = e^{+iT\sigma_i^z\sigma_j^z}$. With this, the problem is reduced to solving

$$e^{-iTH_P^{zz}} = \prod_k U_k e^{-it_k H_S} U_k^\dagger = \prod_k e^{-it_k H_S^{(k)}}, \tag{3}$$

with U_k the digital block at step k containing the X gates, and $H_S^{(k)}$ is the effective source Hamiltonian at step k. In this case, all effective Hamiltonians commute with each other, $[H_S^{(k)}, H_S^{(k')}] = 0\ \forall k, k'$, and thus the equation can be solved exactly by equating the exponents,

$$T \sum_{i<j} h_{P_{ij}}^{zz} \sigma_i^z \sigma_j^z = \sum_k t_k H_S^{(k)} = \sum_k t_k \sum_{i<j} \gamma_{ik}\gamma_{jk} h_{S_{ij}}^{zz} \sigma_i^z \sigma_j^z, \tag{4}$$

where $\gamma_{ik} = -1$ if an X is applied to the ith qubit at the kth step and $\gamma_{ik} = 1$ otherwise. Here, the unknown parameters are the analog block times t_k, as the effective Hamiltonians are fixed by the election of the digital blocks.

We can further rearrange this equation equating both sides term by term. We therefore employ a notation in which we express an arbitrary two-body Hamiltonian, $H = \sum_{i<j}\sum_{\mu,\nu} h_{ij}^{\mu\nu}\sigma_i^\mu\sigma_j^\nu$, by arranging its coupling terms into a matrix $\mathbf{H}$, $\mathbf{H}_{3i+\mu,3j+\nu} = h_{ij}^{\mu\nu}$, with every qubit index i starting at $i = 0$. By using this notation, and by rearranging the Hamiltonian parameters to the right-hand side of the equation, we end up with a simple linear system of equations of the form

$$Mt = T\mathbf{H}_P \oslash \mathbf{H}_S, \tag{5}$$

where M is a tensor representing the changes in the effective Hamiltonians at each step, t is the vector containing the analog block times, and $\oslash$ is the element-wise or Hadamard division. The main goal is to reduce as much as possible the total time to implement the simulation, $t_A \sim \|t\|_1$. As shown in Ref. [17], solving this problem exactly might be exponentially costly, although greedy algorithms tend to provide a solution in polynomial time.

In general, we do not want to restrict ourselves to Hamiltonians of the form given by Eq. (2). Instead, we want to be able to perform the simulation for an arbitrary problem using any given two-body Hamiltonian as a resource.

As a starting point, let us assume a situation in which $h_{S_{ij}}^{\mu\nu} \neq 0$ if $h_{P_{ij}}^{\mu\nu} \neq 0$. In Ref. [17], the proposed DAQC schedules contained digital blocks with all possible combinations of the Pauli gates. This way, the system of equations can be written as

$$T \sum_{i<j}\sum_{\mu,\nu} h_{P_{ij}}^{\mu\nu}\sigma_i^\mu\sigma_j^\nu = \sum_k t_k \sum_{i<j}\sum_{\mu,\nu} \gamma_{ik}^\mu\gamma_{jk}^\nu h_{S_{ij}}^{\mu\nu}\sigma_i^\mu\sigma_j^\nu, \tag{6}$$

where $\mu\nu$ takes the indices of the Pauli gates, $\{\mu, \nu\} \in \{x, y, z\}$. For this initial proposal, γ_{ik}^{μ} could only take values of ± 1. However, a later proposal designed DAQC circuit in which the digital blocks contained combinations of the SQGs in the Clifford group, lifting the requirement for solving the equations when $h_{\mathrm{S}ij}^{\mu\nu} \neq 0$ for at least one combination of $\{\mu, \nu\}$ if $h_{\mathrm{P}ij}^{\mu\nu} \neq 0$ for any $\{\mu, \nu\}$ [16]. In this case, the most general system of equations can be written as

$$T \sum_{i<j} \sum_{\mu,\nu} h_{\mathrm{P}ij}^{\mu\nu} \sigma_i^{\mu} \sigma_j^{\nu} = \sum_k t_k \sum_{i<j} \sum_{\mu,\nu,\xi,\eta} \gamma_{ik}^{\xi\mu} \gamma_{jk}^{\eta\nu} h_{\mathrm{S}ij}^{\xi\eta} \sigma_i^{\mu} \sigma_j^{\nu}, \tag{7}$$

with $\{\xi, \eta\} \in \{x, y, z\}$. However, as the set of gates employed is discrete, we can write these equations in a similar fashion as in Eq. (6) by including the information of the extra components $\{\xi, \eta\}$ in the definition of each block k. There is an additional proposal in Ref. [17] in which arbitrary SQGs can be applied during the digital blocks. This also relaxes the requirements on H_{S}, but it has a drawback. The computational cost of obtaining the optimal SQGs for the circuit is itself a demanding task, as this proposal required constructing an matrix product state (MPS) proxy for evaluating the DAQC circuit. Simulations with MPS will only be efficient in systems satisfying an area law entanglement growth [42], which is far from the general case. As a naive alternative to overcome the requirements for H_{S}, one could also introduce random SQGs, albeit with no guarantees that the obtained t_{A} is optimal [17].

While Eqs. (6) and (7) are always an exact identity, we see that Eq. (3) will not longer be exact when working with arbitrary Hamiltonians, since the effective Hamiltonians do not necessarily commute with each other. Thus, solving this system of equations will not yield the ideal DAQC circuit, as there would be a Trotterization error. As a rule of thumb, we can employ the Lie formula to arbitrarily reduce the errors by dividing the circuit into different steps [3], so that Eq. (3) holds up to a controllable error.

Importantly, from Eq. (7) it follows that the size of the system of equations needed to solve the problem grows with the total number of qubits. Even if we restrict ourselves to suboptimal protocols with polynomially large schedules, we would require large computational resources to obtain a valid DAQC circuit. This is one of the open problems that holds back the scaling of DAQC to systems consisting of a large number of qubits. Thus, there is still the question of whether we can obtain valid DAQC circuits using minimally costly algorithms.

III. CONSTRUCTIVE PROTOCOL FOR HAMILTONIAN SIMULATION

We introduce a new DAQC protocol that relies on an exact solution of Eq. (7) when the source Hamiltonian is of the form given by Eq. (2). Our target is to obtain a valid DAQC circuit for simulating an arbitrary two-body Hamiltonian H_{P} for a given time T on a N qubit system, minimizing computational resources. For that, we will first assume that H_{S} is a ZZ Hamiltonian with compatible topology, i.e. $h_{\mathrm{S}ij}^{zz} \neq 0$ if there is any coupling between qubits i and j in the problem Hamiltonian, $h_{\mathrm{P}ij}^{\mu\nu} \neq 0$ for some μ, ν.

While in previous attempts the usual approach was to define the digital blocks in terms of a finite set of SQGs [16,17,22], here we allow for the implementation of arbitrary SQGs. Therefore, the unitary evolution corresponding to a digital block can be written as

$$U_k = U_{1k} \otimes \cdots \otimes U_{ik} \otimes \cdots \otimes U_{Nk}, \tag{8}$$

where U_{ik} represents an arbitrary single qubit gate for qubit i in the kth DA block. In DAQC, we rely on the conjugation of the analog blocks with the digital blocks. In this case, we can obtain the effective Hamiltonian during a digital-analog block by analyzing its effect on a single qubit:

$$U_{ik} \sigma_i^z U_{ik}^{\dagger} = \gamma_{ik}^x \sigma_i^x + \gamma_{ik}^y \sigma_i^y + \gamma_{ik}^z \sigma_i^z, \tag{9}$$

where the vector $\gamma_{ik} \coloneqq (\gamma_{ik}^x, \gamma_{ik}^y, \gamma_{ik}^z)$ [43] with $-1 \leqslant \gamma_{ik}^{\mu} \leqslant 1$ is normalized with respect to the 2-norm [44]

$$\|\gamma_{ik}\| = \sqrt{\left(\gamma_{ik}^x\right)^2 + \left(\gamma_{ik}^y\right)^2 + \left(\gamma_{ik}^z\right)^2} = 1 \ \ \forall\, i, k, \tag{10}$$

and $\{\gamma_{ik}^x, \gamma_{ik}^y, \gamma_{ik}^z\}$ define the SQG (see Appendix A for more details about the parametrization). With this we can write the effective source Hamiltonian for each block k, and the complete system of equations that follow from Eq. (7). As in the usual DAQC fashion, we can take all constants to the right of the equation, grouping them in a single constant. For convenience, we choose to use the matrix notation

$$\sum_k t_k \gamma_{ik}^{\mu} \gamma_{jk}^{\nu} = T h_{\mathrm{P}ij}^{\mu\nu} \big/ h_{\mathrm{S}ij}^{zz} = \mathbf{B}_{ij}^{\mu\nu}, \ \ \forall\, i \neq j, \mu, \nu, \tag{11}$$

where, in general, $\mathbf{B}$ is a $3N \times 3N$ real matrix. This matrix can be divided into a matrix of $N \times N$ blocks, with each block being a submatrix of size 3×3. The submatrices are associated with the directional couplings between each pair of qubits. Notice that the values of the diagonal submatrices of $\mathbf{B}$ are not fixed, as they are not associated with any physical coupling. Notice also that the matrix $\mathbf{B}$ is symmetric by construction, even in the indeterminate diagonal blocks.

Attempting to solve this equation using classical optimizers is a hard task, specially taking into account that we are facing an optimization problem with $9NK$ variables, where K is the number of digital-analog blocks. In general we do not have a fixed value of K, but for arbitrary problems without symmetries we need at least as many variables as degrees of freedom to solve the equation, requiring $K \geqslant N(N-1)/2$. However, the constraint from Eq. (10) makes it difficult to navigate through the optimization landscape. Convergence of an heuristic approach might not be guaranteed and the computational cost to get a solution might be too high if convergence is not fast enough. Thus, we seek an analytical solution which requires minimal computational resources.

Let us start by noting that $\mathbf{B}$ is a Hermitian matrix, and thus we can obtain its eigendecomposition,

$$\mathbf{B} = \mathbf{U}^{\dagger} \lambda \mathbf{U}, \tag{12}$$

with λ a real diagonal matrix, and $\mathbf{U}$ a real unitary matrix with normalized columns $\vec{v}_l$. Notice that the form of the eigendecomposition of $\mathbf{B}$ is very similar to our problem in Eq. (11), albeit with some important differences.

The first one is that we need positive times for DAQC, so the eigenvalues λ_k should all be positive. If we fix all

indeterminate terms to be zero, the matrix **B** will be indefinite and will have a negative minimum eigenvalue $\tilde{\lambda}_{\min} < 0$. We can make **B** positive-semidefinite if we fix the diagonal to $-\tilde{\lambda}_{\min}$, fixing the off-diagonal indeterminate elements to be zero.

The second difference is complicated to solve. Usually, eigenvectors are given such that they are normalized, $\|\vec{v}_k\| = 1$. However, we ask our vectors $\vec{\gamma}$ to fulfill a different normalization condition given by Eq. (10). In general, there is no rescaling of $\vec{v}$ that will satisfy this condition, as this would require each 3-element block of the vector to have a uniform norm, $\|v_i\| = \|v_j\|\ \forall i \neq j$, which is very unlikely to happen.

Result 1. For an arbitrary two-body Hamiltonian H_{P} and a compatible ZZ Hamiltonian H_{S}, there exists a decomposition of H_{P} which employs a quadratic number of transformations of H_{S} with local unitary gates U_q,

$$TH_{\mathrm{P}} = \sum_{q=1}^{O(N^2)} t_q U_q H_{\mathrm{S}} U_q^{\dagger}, \quad t_q > 0. \tag{13}$$

Calculating this transformation requires only polynomial computational resources.

In other words, there is a decomposition of the matrix **B** with a polynomial number of steps and which employs a construction that only requires SQGs. The main idea behind this construction is to employ a divide and conquer strategy. Instead of focusing on the whole equation, we will search a solution for each of its eigenvectors. This way, we obtain a decomposition of the form

$$\mathbf{B} = \sum_{k=1}^{3N} \lambda_k \vec{v}_k \vec{v}_k^{\dagger} = \sum_{k=1}^{3N} t_k \sum_{\ell=1}^{2N} \left(\vec{\gamma}_{+k}^{(\ell)} \vec{\gamma}_{+k}^{(\ell)\dagger} + \vec{\gamma}_{-k}^{(\ell)} \vec{\gamma}_{-k}^{(\ell)\dagger}\right), \tag{14}$$

with $t_k = \lambda_k \max_i \|v_{ik}\|^2/(4N)$, $\vec{\gamma}_{\pm k}^{(\ell)}$ having components

$$\gamma_{\pm ik}^{(\ell)} = \frac{v_{ik} \pm \varepsilon_{ik}^{(\ell)}}{\sqrt{\|v_{ik}\|^2 + \left\|\varepsilon_{ik}^{(\ell)}\right\|^2}}, \tag{15}$$

and

$$\varepsilon_{ik}^{(\ell)} = \cos\theta_{ik}^{(\ell)} \eta_{ik} + \sin\theta_{ik}^{(\ell)} \xi_{ik}, \tag{16}$$

with $v_{ik} \perp \eta_{ik} \perp \xi_{ik}$, $\|\eta_{ik}\|^2 = \|\xi_{ik}\|^2 = \max_i \|v_{ik}\|^2 - \|v_{ik}\|^2$, and the angles given by

$$\theta_{ik}^{(\ell)} = \frac{\pi(i-1)(\ell-1)}{N} \quad \forall k. \tag{17}$$

Here the selection of the $\varepsilon_{ik}^{(\ell)}$ elements is not unique, but this particular choice allow us to provide a decomposition with $2N$ steps per eigenvalue. Indeed, η_{ik} and ξ_{ik} can take any particular value as long as they fulfill the conditions, and so are left as free parameters. Note here that the complexity of this construction is polynomial in time, as the computational cost is $O(N^3)$, corresponding to the cost of the eigendecomposition of the problem matrix **B**. A constructive proof is given in Appendix B.

The decomposition we have shown can be straightforwardly employed to generate a DAQC protocol for simulating H_{P}. Since we already have the analog block times, all we need to do is to extract information about the SQGs from the $\vec{\gamma}$ vectors. This depends on the particular choice parametrizing arbitrary SQGs. In Appendix A, we show how to extract the angles of rotation for one particular SQG parametrization. With this, the DAQC circuit is

$$e^{-iTH_{\mathrm{P}}} \approx \prod_q U_q e^{-it_q H_{\mathrm{S}}} U_q^{\dagger} = \prod_q e^{-it_q H_{\mathrm{S}}^{(q)}}, \tag{18}$$

with the index q running over the indices employed in Eq. (14). The derivation of the DAQC circuit is shown in Appendix C.

It is important to note that the target evolution operator and the one obtained from the DAQC circuit are not equal. Hence, we have a Trotter error comming from the decomposition of H_{P} into noncommuting terms. As it is usual in such decompositions and DAQC, one can always use the Lie formula to divide the evolution into n_{T} steps to reduce Trotterization errors. However, this might not be technically viable, as we would increase the number of digital-analog blocks by n_{T} while also reducing the time of the analog block times by t_k/n_{T}.

All in all, the DAQC circuit is composed of a maximum of $12N^2$ digital-analog blocks, which is in the same order of magnitude as the ones required in previous protocols [16,17,22]. Also, the expression of the analog block times allows us to easily bound the total analog block time in terms of the eigenvalues of **B**,

$$t_{\mathrm{A}} \leqslant \sum_k \lambda_k = \mathrm{tr}(\mathbf{B}) = 3N|\tilde{\lambda}_{\min}|. \tag{19}$$

Additionally, this protocol gives us an immediate method for discarding negligible terms [5,17]. In particular, we can discard the simulation corresponding to the kth eigenvector if the associated analog time t_k is below certain threshold.

IV. NUMERICAL CALCULATIONS

Here we show results on the calculations performed to verify the scalability of our approach. For that, first we have to generate valid problems. In our case, we have chosen to generate **B** directly, without connecting it to any particular problem nor source Hamiltonians. For our tests, we have generated these matrices with a random uniform distribution on the range $-1 \leqslant \mathbf{B}_{3i+\mu,3j+\nu} \leqslant 1$. This ensures that the generated matrices represent systems without symmetries or other exploitable features, thus corresponding to the worst possible case for DAQC compilation. We further normalize our matrices such that the maximum magnitude of any element is 1, i.e., $\max|\mathbf{B}_{3i+\mu,3j+\nu}| = 1$. With these problem matrices, we have computed the total analog block times t_{A} obtained using the construction outlined in Result 1.

In Fig. 2, we represent t_{A} as a function of the total number of qubits N, up to systems of size $N = 50$. For each value of N, we have generated 10^4 random **B** matrices. In the figure, we show the obtained total time, and the upper bound given by Eq. (19). In order to compare this protocol against previous ones, we also represent the obtained upper bound of t_{A} for an optimal DAQC protocol as provided in Ref. [45], in this case $t_{\mathrm{A}} \leqslant \sqrt{3}(\sum_{i<j} \mathbf{B}_{i,j}^2)^{1/2}$ with the elements in the diagonal blocks equal to 0.

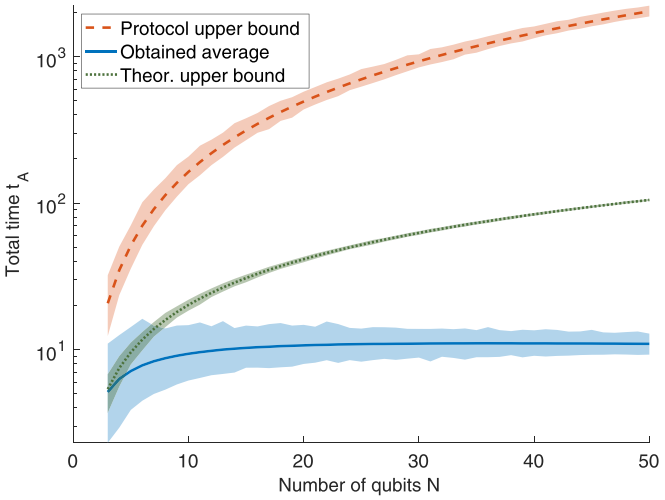

FIG. 2. $\log_{10} t_A$ for random problems of size N. The problem matrices $\mathbf{B}$ are generated with uniform values in the range $[-1, 1]$ and then normalized with the elementwise infinite norm. The solid line shows the average obtained over 10^4 runs. The dashed line shows the upper bound calculated as $t_A \leqslant 3N|\tilde{\lambda}_{\min}|$. The dotted line represents the theoretical upper bound for the optimal DAQC protocol with the Pauli gates. The colored regions represent the area between the maximum and minimum values obtained.

Figure 2 shows that using this normalization of $\mathbf{B}$, t_A scales nearly constant with system size. If we compare both upper bounds, we see that the upper bound for this protocol is significantly larger than the theoretical upper bound for optimal DAQC protocols. This is expected, as the protocol provided in this work is suboptimal and penalizes the optimal upper bound by some factor. Nevertheless, this factor seems to increase slower than linearly with the number of qubits. Additionally, we observe that the obtained t_A grows linearly with the maximum magnitude of the ratio between the problem and the source Hamiltonians, $t_A \sim T \max |\mathbf{B}_{3i+\mu,3j+\nu}| = T \max |h_{P_{ij}}^{\mu\nu} \oslash h_{S_{ij}}^{\mu\nu}|$. In this case, as this value is chosen to be constant, Fig. 2 flattens as N grows.

Although we have not studied extreme cases in which the upper bound for t_A saturates, and our numerical calculations focused on a specific distribution of problems, we expect usual DAQC compilation tasks to involve problem matrices $\mathbf{B}$ following a distribution of their elements similar to the one employed here.

V. CONCLUSIONS

The main result of this paper provides a systematic way to obtain decompositions of arbitrary two-body Hamiltonians using a set of local unitary transformations applied to a ZZ Hamiltonian. This approach allows one to obtain a DAQC protocol employing minimal computational resources, providing a recipe-based method to design DAQC circuits that simulate unitary evolution under arbitrary two-body Hamiltonians. In contrast to previous approaches where solving a hard optimization problem at the preprocessing stage is necessary, the protocol presented in this work eliminates this requirement by making use of exact expressions. Indeed, we have shown that the original problem can be brought into a form similar to eigendecomposition of a $3N \times 3N$ positive semidefinite matrix, with N the number of qubits, thus yielding a runtime polynomial with system size $O(N^3)$. Additionally, the proposed protocol yields DAQC circuits composed of at most $12N^2$ digital-analog blocks, which is in the same order of magnitude as previous protocols that required up to $9N(N-1)/2$ blocks. Even though the presented protocol is suboptimal in terms of total analog block time $t_A = \sum_q t_q$, the numerical calculations reported here show that this value does not grow with N for problems in which the ratio between the problem and the source Hamiltonian couplings is bounded, suggesting a relation $t_A \sim T \max |h_{P_{ij}}^{\mu\nu} \oslash h_{S_{ij}}^{\mu\nu}|$. These results contribute to a favorable scaling of DAQC protocols for systems consisting of a large number of qubits, in this case by lowering the classical computational resources needed for compiling such circuits.

Although the protocol presented here relies on source Hamiltonians having only ZZ terms, this can be easily extended to Hamiltonians with symmetric terms (i.e., Hamiltonians with XX or YY terms). For generic source Hamiltonians, one could first obtain an effective ZZ Hamiltonian from the protocol by interchanging the roles of H_S and H_P, and then apply the protocol again to simulate the problem of interest. However, this would introduce a large overhead in the number of required blocks [46]. Extension of the protocol to efficiently employ arbitrary source Hamiltonians as those in Eq. (7) is still an open question.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this paper. Requests for further information or data should be sent to the authors.

APPENDIX A: SQG PARAMETRIZATION

Several parametrizations can be chosen for the SQGs. Here, we define an arbitrary single qubit rotation as

$$R(\theta, \hat{n}) = e^{-i\frac{\theta}{2}(n_x\sigma^x + n_y\sigma^y + n_z\sigma^z)}, \tag{A1}$$

where $\hat{n} = (n_x, n_y, n_z)$ is a unit vector. This operator can be employed to construct each of the local unitaries in Eq. (8);

we have omitted the qubit index to ease the notation. Applying this arbitrary rotation to Eq. (9), we obtain the following identities:

$$\gamma^x = n_x n_z[1-\cos(\theta)] + n_y \sin(\theta),$$
$$\gamma^y = n_y n_z[1-\cos(\theta)] - n_x \sin(\theta),$$
$$\gamma^z = n_z^2[1-\cos(\theta)] + \cos(\theta). \tag{A2}$$

Note that, due to the normalization condition $\sqrt{n_x^2+n_y^2+n_z^2}=1$, there are three degrees of freedom for a single arbitrary rotation. Further note that here we can choose $n_z = 0$, simplifying the identities.

APPENDIX B: PROOF OF MAIN RESULT

In this Appendix we give a proof for Result 1. For that, we will construct step by step a decomposition for any problem **B** as given in Eq. (11).

As we have seen in the main text, we can always write the problem as a positive semi-definite matrix by giving a value to the indeterminate terms in the diagonal blocks. This way, our goal is to find a decomposition of the form

$$\mathbf{B} = \sum_{k=1}^{3N} \lambda_k \vec{v}_k \vec{v}_k^\dagger = \sum_{q=1}^{Q} t_q \vec{\gamma}_q \vec{\gamma}_q^\dagger, \tag{B1}$$

with $\lambda_k \geqslant 0$ the eigenvalues corresponding to the eigenvector $\vec{v}_k$, $t_q > 0$, and $\vec{\gamma}_q$ subjected to the normalization condition given in Eq. (10). In the presence of degenerate eigenvalues, the corresponding eigenvectors v_k should be chosen such that their corresponding $\|v_i\|$ is nonzero such that the normalization condition can be met.

Instead of focusing on the whole equation, we will search a solution for each of the eigenvector projectors,

$$\lambda \vec{v}\vec{v}^\dagger = \sum_{\ell=1}^{L} t^{(\ell)} \vec{\gamma}^{(\ell)} \vec{\gamma}^{(\ell)\dagger}, \tag{B2}$$

where we have dropped the index k for easier notation.

As an initial guess, we consider $\vec{\gamma}^{(\ell)}$ vectors consisting of different blocks given by the eigenvector components plus some perpendicular perturbation $\varepsilon_i^{(\ell)} \perp v_i$ and which fulfill Eq. (10),

$$\gamma_i^{(\ell)} = \frac{v_i + \varepsilon_i^{(\ell)}}{\left\| v_i + \varepsilon_i^{(\ell)} \right\|} = \frac{v_i + \varepsilon_i^{(\ell)}}{\sqrt{\|v_i\|^2 + \left\|\varepsilon_i^{(\ell)}\right\|^2}}. \tag{B3}$$

As it is not possible to solve Eq. (B2) with a single step, we begin with two steps. This way, for each $i \neq j$ we have

$$\lambda v_i v_j^\dagger = t^{(1)} \gamma_i^{(1)} \gamma_j^{(1)\dagger} + t^{(2)} \gamma_i^{(2)} \gamma_j^{(2)\dagger}. \tag{B4}$$

In order to make the equation simpler, we choose to cancel the crossed terms resulting from $v_i \varepsilon_j^{(\ell)}$ and $\varepsilon_i^{(\ell)} v_j$ by selecting the vectors such that $\vec{\varepsilon}^{(1)} = -\vec{\varepsilon}^{(2)} = \vec{\varepsilon}$. This fixes the election of the times to cancel the crossed terms, $t^{(1)} = t^{(2)} = t$. Let us further impose that $\|v_i\|^2 + \|\varepsilon_i\|^2 = \|v_j\|^2 + \|\varepsilon_j\|^2 \; \forall i \neq j$. This choices leaves us with

$$\lambda v_i v_j^\dagger = \frac{2t}{\|v_i\|^2 + \|\varepsilon_i\|^2} (v_i v_j^\dagger + \varepsilon_i \varepsilon_j^\dagger). \tag{B5}$$

This equation suggests fixing the analog block times and the norms such that

$$\|v_i\|^2 + \|\varepsilon_i\|^2 = \frac{2t}{\lambda} \;\; \forall i. \tag{B6}$$

From this equation for two steps, we can extract a lower bound on the analog block times, $t \geqslant \lambda \max_i \|v_i\|^2/2$. As we would like to minimize the total circuit time, we can set the value of t to this limiting value. This fixes the norms of all ε_i vectors to $\|\varepsilon_i\|^2 = \max_i \|v_i\|^2 - \|v_i\|^2$.

Up to this point, we have obtained an approximation of $\lambda \vec{v}\vec{v}^\dagger$ with an error of $\lambda \vec{\varepsilon}\vec{\varepsilon}^\dagger$. This hints toward employing more steps in order to obtain an exact expansion of our target. In doing so, we will construct pairs of blocks in which we select the $\vec{\varepsilon}^{(\ell)}$ vectors in the way discussed previously for L different contributions. The decomposition takes the form

$$\lambda v_i v_j^\dagger = \sum_{\ell=1}^{L} \frac{2t^{(\ell)}}{\|v_i\|^2 + \left\|\varepsilon_i^{(\ell)}\right\|^2} \left(v_i v_j^\dagger + \varepsilon_i^{(\ell)} \varepsilon_j^{(\ell)\dagger}\right), \tag{B7}$$

with $\varepsilon_i^{(\ell)} \perp v_i$. Now, we take an extra choice by setting all times to be equal, $t^{(\ell)} = t$. This way, we fix the norms of the vectors for all steps, $\|\varepsilon_i^{(\ell)}\| = \|\varepsilon_i\|$. For a total of L steps, we take $t = \lambda \max_i \|v_i\|^2/(2L)$ to fix the equality on the $v_i v_j^\dagger$ terms.

The last step to fulfill the identity in Eq. (B7) is to fix the remaining free parameters. For that, we expand the rightmost term of Eq. (B7) to the the following system of equations:

$$\sum_{\ell=1}^{L} \varepsilon_i^{(\ell)} \varepsilon_j^{(\ell)\dagger} = 0_{3,3} \; \forall i \neq j. \tag{B8}$$

Since we have previously fixed the norm of these vectors and the plane they live in, we can parametrize them with a single parameter:

$$\varepsilon_i^{(\ell)} = \cos\theta_i^{(\ell)} \eta_i + \sin\theta_i^{(\ell)} \xi_i, \tag{B9}$$

such that $v_i \perp \eta_i \perp \xi_i$, $\|\varepsilon_i\| = \|\eta_i\| = \|\xi_i\|$, and $\theta_i^{(\ell)} \in [0, 2\pi)$. Note here that these conditions can be satisfied even in the cases in which $v_i = 0$, as in this case we can consider that any vector is orthogonal to it, $\vec{0} \perp \vec{a} \;\; \forall \vec{a}$. Here, we have freedom for selecting any auxiliary vectors η_i and ξ_i at qubit i that fulfill these conditions. An easy analytical solution to this system of equations with a number of steps $L = 2N$ [48] is found by choosing

$$\theta_i^{(\ell)} = \frac{\pi(i-1)(\ell-1)}{N}. \tag{B10}$$

This way, we can build the decomposition of the matrix **B** shown in Eq. (14).

APPENDIX C: FROM THE DECOMPOSITION OF B TO THE DAQC CIRCUIT

In this Appendix we show how to construct the DAQC circuit that simulates the evolution under H_{P} by employing the decomposition from Eq. (14).

We start from the definition of the matrix $\mathbf{B}$ given in Eq. (11), and we isolate the couplings from the problem Hamiltonian,

$$T h_{\mathrm{P}_{ij}}^{\mu\nu} = h_{\mathrm{S}_{ij}}^{zz} \mathbf{B}_{ij}^{\mu\nu} \quad \forall\, i \neq j,\, \mu,\, \nu. \tag{C1}$$

Now, we can substitute the expression from Eq. (14),

$$T h_{\mathrm{P}_{ij}}^{\mu\nu} = h_{\mathrm{S}_{ij}}^{zz} \sum_{k=1}^{3N} t_k \sum_{\ell=1}^{2N} \left(\vec{\gamma}_{+ik}^{(\ell)\mu} \vec{\gamma}_{+jk}^{(\ell)\nu} + \vec{\gamma}_{-ik}^{(\ell)\mu} \vec{\gamma}_{-jk}^{(\ell)\nu} \right) = \sum_q t_q h_{\mathrm{S}_{ij}}^{\mu\nu(q)}, \tag{C2}$$

where $h_{\mathrm{S}_{ij}}^{\mu\nu(q)}$ is the effective coupling of the source Hamiltonian at the qth step. Adding the corresponding Pauli terms and summing over all indices, we can write the equation corresponding to the decomposition of the problem Hamiltonian as in Eq. (7),

$$\begin{aligned} T H_{\mathrm{P}} &= T \sum_{i<j} \sum_{\mu,\nu} h_{\mathrm{P}_{ij}}^{\mu\nu} \sigma_i^\mu \sigma_j^\nu = \sum_{k=1} t_k H_{\mathrm{P}}^{(k)} = \sum_{i<j} \sum_{\mu,\nu} h_{\mathrm{S}_{ij}}^{zz} \sum_{\eta=\{+,-\}} \sum_{k=1}^{3N} t_k \sum_{\ell=1}^{2N} \vec{\gamma}_{\eta ik}^{(\ell)\mu} \vec{\gamma}_{\eta jk}^{(\ell)\nu} \sigma_i^\mu \sigma_j^\nu \\ &= \sum_q t_q U_q H_{\mathrm{S}} U_q^\dagger = \sum_q t_q H_{\mathrm{S}}^{(q)}. \end{aligned} \tag{C3}$$

The last step is employ Eq. (9) to obtain the local unitary rotations U_q giving the effective Hamiltonian. A mapping like the one described in Appendix A can be used to obtain the parameters of the single qubit gates generating each effective Hamiltonian. With this, we arrive at the expression shown in Eq. (18).

We stress that the gauge invariance employed here to rewrite the matrix $\mathbf{B}$ as a positive semidefinite matrix has no effect in the overall Hamiltonian decomposition. This is because indeterminate values of $\mathbf{B}$ correspond to two equal qubit indices. Since these do not correspond to two-body terms, changing these indeterminate values does not alter the description of the original problem.

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[43] As a visual key, we will denote with the vector mark $\vec{\cdot}$ the vectors with size $3N$, in contrast to the vectors of size 3, which will be written without it.

[44] 2-norm or Euclidean norm, which is $v \in \mathbb{R}^n$, $\|v\|_2 = (\sum_{i=1}^n v_i^2)^{1/2}$. As this is the only vector norm that we employ in this paper, we omit the subindex.

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[46] As we would need to obtain an effective ZZ Hamiltonian for each block, we would have a total number of blocks in the order of $O(N^4)$.

[47] IQDA, https://qci.dlr.de/projects/IQDA.

[48] As a fun fact, if we wanted to solve this equation with the optimum amount of steps, there is another analytical solution which employs N steps if N is a power of 2. In this case, we can associate the matrix $\vec{\varepsilon}\vec{\varepsilon}^\dagger$ with the $n \times n$ Hadamard matrix, as its definition coincides with Eq. (B8) for all off-diagonal 3×3 blocks.