

Quantum wave simulation with sources and loss functions

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We present a quantum algorithmic framework for simulating linear, anti-Hermitian (lossless) wave equations in heterogeneous, anisotropic, and time-independent media. This framework encompasses a broad class of wave equations, including the acoustic wave equation, Maxwell's equations, and the elastic wave equation. Our formulation is compatible with standard numerical discretization schemes and allows for the efficient implementation of multiple practically relevant time- and space-dependent sources. Furthermore, we demonstrate that subspace energies can be extracted and wave fields compared through an l_2 loss function, achieving optimal precision scaling with the number of samples taken. Additionally, we introduce techniques for incorporating boundary conditions and linear constraints that preserve the anti-Hermitian nature of the equations. Leveraging the Hamiltonian simulation algorithm, our framework achieves a quartic speedup over classical solvers in three-dimensional simulations, under conditions of sufficiently global measurements and compactly supported sources and initial conditions. This quartic speedup is optimal for time-domain solutions, as the Hamiltonian of the discretized wave equations has local couplings. In summary, our framework provides a versatile approach for simulating wave equations on quantum computers, offering substantial speedups over state-of-the-art classical methods.

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I. INTRODUCTION

Wave-based inverse problems are prevalent in disciplines such as seismology [1–4], medical imaging [5–7], nondestructive testing [8–10] and metamaterial research [11–14]. However, these fields are fundamentally limited by the current state of computational resources due to the excessive computational cost of the numerical wave simulation. In particular, resolution and uncertainty quantification in imaging problems remain heavily restricted by computational capacities [15–21].

Quantum computers (QCs) offer promising runtime improvements for numerous computational problems [22–25]. One of the most promising groups of quantum algorithms is Hamiltonian simulation (HS). It provides a framework for simulating quantum systems, i.e., the evolution of the Schrödinger equation, with up to exponential runtime advantages over classical solvers [26–29]. A quantum state represented by n two-state quantum particles or qubits has

a state space dimension of $N = 2^n$. Classical algorithms for simulating the evolution of a quantum state under a quantum Hamiltonian $\mathbf{H} \in \mathbb{C}^{N \times N}$ scale at least linearly with the state size N . In contrast, under specific conditions utilizing HS algorithms, a QC is capable of performing quantum simulations with logarithmic scaling, thereby achieving an exponential speedup compared to all classical computers. This can be formalized as follows:

Theorem 1 (Optimal sparse Hamiltonian simulation, adapted from Ref. [27], Theorem 3). A d -sparse Hamiltonian $\mathbf{H}$ acting on n qubits with matrix elements specified to m bits of precision can be simulated for time interval T , l_2 error ϵ , and success probability at least $1 - 2\epsilon$ with $O(Td\|\mathbf{H}\|_{\max} + \frac{\log(1/\epsilon)}{\log \log(1/\epsilon)})$ queries to an oracle $\mathcal{H}$ that provides a description of $\mathbf{H}$ and a factor $O(n + m \text{ polylog}(m))$ additional quantum gates.

The apparent question is as follows: Can HS algorithms be used to simulate classical wave equations with the same runtime advantages? A growing body of research answers this question affirmatively. These studies examine source-free wave equations in homogeneous media [30,31] or wave equations in media with varying parameters [32–35]. Furthermore, recent research has investigated solutions to mass-spring models [36,37] that yield exponential runtime advantages in certain settings, with particular types of source terms considered in Ref. [38], or wave simulation problems addressed through warped phase transformations [39–41].

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While many existing studies tend to focus on simulation tasks, our research expands the scope to address the complete end-to-end stack by incorporating a wide range of practically relevant source scenarios and loss function measurements. We thoroughly analyze the conditions necessary to preserve quantum speedup throughout the entire algorithmic stack. Our primary result is to demonstrate that for many practically relevant sources that are either compact or rotationally symmetric, and when the measured quantities of the final state have sufficiently global characteristics relative to the system size, the proposed algorithmic framework achieves a quartic speedup in the three-dimensional (3D) case compared to all classical wave equation solvers.

The rest of the paper is organized as follows. In Sec. II, we demonstrate that for lossless wave equations, including the elastic, acoustic, and electromagnetic cases, a natural quantum encoding can be employed, which enables a direct measurement of the wave field energy and l_2 norms. We then analyze the runtime advantage for time-domain solutions of wave equations (Sec. III). In Sec. IV, we introduce algorithms to measure l_2 -related norms and subspace energies for extracting information from the simulated wave field. Then, we propose a method for the implementation of sources on a QC (Sec. V). Finally, we analyze the limitations of our framework (Sec. VI) and draw conclusions (Sec. VII).

II. A NATURAL QUANTUM ENCODING FOR LINEAR, ANISOTROPIC, HETEROGENEOUS BUT LOSSLESS WAVE EQUATIONS

We consider continuous wave equations of the form

$$\begin{aligned} \frac{d\hat{\mathbf{w}}(\mathbf{x}, t)}{dt} &= \hat{\mathbf{C}}(\mathbf{x})\hat{\mathbf{w}}(\mathbf{x}, t) + \hat{\mathbf{s}}(\mathbf{x}, t), \\ \hat{\mathbf{w}}(\mathbf{x}, 0) &= \hat{\mathbf{w}}_0(\mathbf{x}), \\ \hat{\mathbf{P}}_{\partial\Omega}\hat{\mathbf{w}}(\mathbf{x}, t) &= \mathbf{0}, \forall \mathbf{x} \in \partial\Omega, \end{aligned} \quad (1)$$

where hats ($\hat{\cdot}$) denote continuous fields and operators over D -dimensional space, $\mathbf{x} \in \mathbb{R}^D$, and time t . The wave field $\hat{\mathbf{w}}$ is an element of a Hilbert space $\mathcal{H} = \{f : \mathbb{R}^D \rightarrow \mathbb{R}^C\}$ containing at least once-differentiable (in both space and time) and square-integrable C -dimensional vector fields over the domain Ω , and $\hat{\mathbf{s}}$ is the source term. For concreteness and without loss of generality, we have chosen Dirichlet boundary conditions (BCs) on the domain boundary $\partial\Omega$, where $\hat{\mathbf{P}}_{\partial\Omega} \in \mathcal{B}(\mathcal{H})$ is a diagonal projector, which selects the elements of the wave field on which we impose homogeneous Dirichlet BC.

The wave operator $\hat{\mathbf{C}}$ considered here is assumed to have the following form:

$$\hat{\mathbf{C}} := \hat{\mathbf{B}}^{-1}(\mathbf{x})\hat{\mathbf{A}}(\mathbf{x}), \quad (2)$$

where $\hat{\mathbf{B}} : \mathcal{H} \rightarrow \mathcal{H}$ is any Hermitian (self-adjoint) and positive-definite operator, and $\hat{\mathbf{A}} : \mathcal{H} \rightarrow \mathcal{H}$ is any anti-Hermitian (anti-self-adjoint) operator with respect to the inner product

$$\langle \hat{\mathbf{w}} | \hat{\mathbf{w}}' \rangle_{\mathbf{B}} := \int_{\Omega} \langle \hat{\mathbf{w}}(\mathbf{x}, t) | \hat{\mathbf{w}}'(\mathbf{x}, t) \rangle d\mathbf{x}, \quad (3)$$

where $\langle \hat{\mathbf{w}} | \hat{\mathbf{w}}' \rangle = \sum_{l=1}^L \hat{w}_l^* \hat{w}'_l$, $(*)$ denotes complex conjugation, and $\hat{\mathbf{w}}, \hat{\mathbf{w}}' \in \mathcal{H}$ are any two vector fields. Here, $\hat{\mathbf{A}}$

incorporates various types of spatial derivatives such as divergence, gradient, or curl operations. The operator $\hat{\mathbf{C}}$ is therefore anti-Hermitian with respect to the inner product

$$(\hat{\mathbf{w}} | \hat{\mathbf{w}}')_{\mathbf{B}} := \int_{\Omega} \langle \hat{\mathbf{w}}(\mathbf{x}, t) | \hat{\mathbf{B}}(\mathbf{x}) | \hat{\mathbf{w}}'(\mathbf{x}, t) \rangle d\mathbf{x}, \quad (4)$$

where

$$\langle \hat{\mathbf{w}}(\mathbf{x}, t) | \hat{\mathbf{B}}(\mathbf{x}) | \hat{\mathbf{w}}'(\mathbf{x}, t) \rangle = \sum_{l=1}^L \sum_{m=1}^L \hat{w}_l^*(\mathbf{x}, t) \hat{B}_{l,m}(\mathbf{x}) \hat{w}'_m(\mathbf{x}, t). \quad (5)$$

As we will discuss shortly, the inner product in Eq. (4) gives rise to a notion of energy that can be estimated on a QC. The anti-Hermiticity of $\hat{\mathbf{C}}$ with respect to $(\cdot | \cdot)_{\mathbf{B}}$ is formalized by showing that

$$(\hat{\mathbf{w}} | \hat{\mathbf{C}} \hat{\mathbf{w}}')_{\mathbf{B}} = -(\hat{\mathbf{C}} \hat{\mathbf{w}} | \hat{\mathbf{w}}')_{\mathbf{B}}, \quad (6)$$

using integration by parts and invoking the BC [35,42]. Quantum states are naturally normalized with respect to a norm induced by the inner product (3). Therefore, mapping Eq. (1) to a Schrödinger equation amounts to transforming $\hat{\mathbf{C}} \rightarrow \hat{\mathbf{C}}_Q$, such that $\hat{\mathbf{C}}_Q$ is anti-Hermitian with respect to $(\cdot | \cdot)_{\mathbf{1}}$ [32,43]. Because $\hat{\mathbf{B}}$ is Hermitian and positive definite, it has a unique square root $\hat{\mathbf{B}}^{1/2}$, which is also Hermitian and positive definite. Transforming Eq. (1) with $\hat{\mathbf{w}}_Q := \hat{\mathbf{B}}^{1/2} \hat{\mathbf{w}}$ and $\hat{\mathbf{C}}_Q := \hat{\mathbf{B}}^{-1/2} \hat{\mathbf{A}} \hat{\mathbf{B}}^{-1/2}$ leads to

$$\begin{aligned} \frac{d\hat{\mathbf{w}}_Q(\mathbf{x}, t)}{dt} &= \hat{\mathbf{B}}^{-1/2}(\mathbf{x}) \hat{\mathbf{A}}(\mathbf{x}) \hat{\mathbf{B}}^{-1/2}(\mathbf{x}) \hat{\mathbf{w}}_Q(\mathbf{x}, t), \\ \hat{\mathbf{w}}_Q(\mathbf{x}, 0) &= \hat{\mathbf{B}}^{1/2}(\mathbf{x}) \hat{\mathbf{w}}_0(\mathbf{x}), \\ \hat{\mathbf{B}}^{1/2}(\mathbf{x}) \hat{\mathbf{P}}_{\partial\Omega} \hat{\mathbf{w}}_Q(\mathbf{x}, t) &= \mathbf{0}, \quad \forall \mathbf{x} \in \partial\Omega. \end{aligned} \quad (7)$$

We ignore the source term here, as it can be incorporated into the initial conditions or handled separately, as we will show in Sec. V. Clearly, because $\hat{\mathbf{A}}$ is anti-Hermitian with respect to $(\cdot | \cdot)_{\mathbf{1}}$, it follows that $\hat{\mathbf{C}}_Q = \hat{\mathbf{B}}^{-1/2} \hat{\mathbf{A}} \hat{\mathbf{B}}^{-1/2}$ is also anti-Hermitian with respect to the same inner product. Multiplying Eq. (7) by the imaginary unit i , we obtain a Schrödinger equation with the corresponding Hamiltonian

$$\hat{\mathbf{H}}(\mathbf{x}) = i\hat{\mathbf{C}}_Q(\mathbf{x}) = i\hat{\mathbf{B}}^{-1/2}(\mathbf{x}) \hat{\mathbf{A}}(\mathbf{x}) \hat{\mathbf{B}}^{-1/2}(\mathbf{x}). \quad (8)$$

Finally, we observe that

$$(\hat{\mathbf{w}} | \hat{\mathbf{w}}')_{\mathbf{B}} = (\hat{\mathbf{w}}_Q | \hat{\mathbf{w}}'_Q)_{\mathbf{1}}. \quad (9)$$

Therefore, if $(\cdot | \cdot)_{\mathbf{B}}$ induces a norm related to the energy of the system, so does $(\cdot | \cdot)_{\mathbf{1}}$ on the transformed states.

A. The acoustic wave equation

For acoustics in D space dimensions, we have that $\hat{\mathbf{w}}_{\text{acoustic}} = [\hat{u}; \hat{\mathbf{v}}] \in \{f : \mathbb{R}^D \rightarrow \mathbb{R}^{D+1}\}$, where $\hat{u}$ is the scalar pressure field and $\hat{\mathbf{v}}$ is the particle velocity field. The respective operators are given by [44]

$$\hat{\mathbf{B}}_{\text{acoustic}}(\mathbf{x}) = \begin{bmatrix} \frac{1}{\rho(\mathbf{x})c^2(\mathbf{x})} & \mathbf{0}_{1 \times D} \\ \mathbf{0}_{D \times 1} & \rho(\mathbf{x})\mathbb{1}_{D \times D} \end{bmatrix}, \quad (10)$$

where $c, \rho \in \{f : \mathbb{R}^D \rightarrow \mathbb{R}\}$ are the wave speed and density, respectively. The anti-Hermitian operator is given by

$$\hat{\mathbf{A}}_{\text{acoustic}} = \begin{bmatrix} 0 & -\nabla \cdot \\ -\nabla & \mathbf{0}_{D \times D} \end{bmatrix}. \quad (11)$$

The inner product relates to the sound energy as

$$\begin{aligned} (\hat{\mathbf{w}}|\hat{\mathbf{w}})_{\hat{\mathbf{B}}}(t) &= \int_{\Omega} \frac{\hat{u}^2(\mathbf{x}, t)}{\rho(\mathbf{x})c^2(\mathbf{x})} d\mathbf{x} + \int_{\Omega} \langle \hat{\mathbf{v}}(\mathbf{x}, t) | \hat{\mathbf{v}}(\mathbf{x}, t) \rangle \rho(\mathbf{x}) d\mathbf{x} \\ &= 2E_{\text{potential}}(t) + 2E_{\text{kinetic}}(t). \end{aligned} \quad (12)$$

B. Maxwell's equations

For Maxwell's equations in D dimensions, the state vector is defined as $\hat{\mathbf{w}}_{\text{Maxwell}} = [\hat{\mathbf{E}}; \hat{\mathbf{H}}] \in \{f : \mathbb{R}^D \rightarrow \mathbb{R}^{2D}\}$, where $\hat{\mathbf{E}}$ represents the electric field and $\hat{\mathbf{H}}$ represents the magnetic field. The operator containing the material properties is given by [42,45]

$$\hat{\mathbf{B}}_{\text{Maxwell}}(\mathbf{x}) = \begin{bmatrix} \boldsymbol{\epsilon}(\mathbf{x}) & \mathbf{0}_{D \times D} \\ \mathbf{0}_{D \times D} & \boldsymbol{\mu}(\mathbf{x}) \end{bmatrix}, \quad (13)$$

where $\boldsymbol{\epsilon}$ and $\boldsymbol{\mu}$ are the generally complex but Hermitian dielectric permittivity and magnetic permeability tensors, respectively. These tensors reduce to a single coefficient multiplied with the identity for isotropic materials. For the presented framework to be applicable, both must be positive definite and Hermitian, thereby specifying a generally anisotropic but transparent medium without any losses [46].

We can further identify the anti-Hermitian operator

$$\hat{\mathbf{A}}_{\text{Maxwell}} = \begin{bmatrix} \mathbf{0}_{D \times D} & \nabla \times \\ -\nabla \times & \mathbf{0}_{D \times D} \end{bmatrix}, \quad (14)$$

where $\nabla \times$ is the curl operator. Finally, the inner product induced norm, which is related to the electromagnetic energy, can be identified as [47]

$$\begin{aligned} (\hat{\mathbf{w}}|\hat{\mathbf{w}})_{\hat{\mathbf{B}}} &= \int_{\Omega} \langle \hat{\mathbf{E}}(\mathbf{x}, t) | \boldsymbol{\epsilon}(\mathbf{x}) | \hat{\mathbf{E}}(\mathbf{x}, t) \rangle d\mathbf{x} \\ &\quad + \int_{\Omega} \langle \hat{\mathbf{H}}(\mathbf{x}, t) | \boldsymbol{\mu}(\mathbf{x}) | \hat{\mathbf{H}}(\mathbf{x}, t) \rangle d\mathbf{x} \\ &= 2E_{\text{electric}}(t) + 2E_{\text{magnetic}}(t). \end{aligned} \quad (15)$$

A final remark concerns the charge density $\rho(\mathbf{x})$ and its implications via Gauss's law. When $\rho(\mathbf{x}) \neq 0$, the corresponding initial electric field is generally neither sparse nor symmetric, so its preparation may become prohibitively expensive. Moreover, if no analytic or precomputed $\mathbf{E}(\mathbf{x}, 0)$ is available for a given $\rho(\mathbf{x})$, one must solve the Poisson equation numerically to obtain $\mathbf{E}(\mathbf{x}, 0)$. In certain cases, however, the Poisson problem can be solved efficiently on a quantum computer [48,49].

C. The elastic wave equation

In the interest of a clear notation, we consider the linear elastic wave equation in 3D. Here, the state vector is given by $\hat{\mathbf{w}}_{\text{elastic}} = [\hat{\mathbf{v}}; \text{vec}(\hat{\boldsymbol{\sigma}})] \in \{f : \mathbb{R}^3 \rightarrow \mathbb{R}^9\}$, where $\hat{\mathbf{v}}$ is the particle velocity field and $\text{vec}(\hat{\boldsymbol{\sigma}}) = [\sigma_{xx}; \sigma_{yy}; \sigma_{zz}; \sigma_{xy}; \sigma_{xz}; \sigma_{yz}]$ denotes the six independent entries of the positive-definite and symmetric stress tensor $\hat{\boldsymbol{\sigma}}$. The corresponding strain tensor can be represented as $\text{vec}[\hat{\boldsymbol{\epsilon}}] = [\epsilon_{xx}; \epsilon_{yy}; \epsilon_{zz}; 2\epsilon_{xy}; 2\epsilon_{xz}; 2\epsilon_{yz}]$. This

notation allows us to represent the constitutive relations in the Voigt notation as [50]

$$\text{vec}[\hat{\boldsymbol{\epsilon}}](\mathbf{x}, t) = \mathbf{S}(\mathbf{x}) \text{vec}[\hat{\boldsymbol{\sigma}}](\mathbf{x}, t), \quad (16)$$

where $\mathbf{S} \in \{f : \mathbb{R}^3 \rightarrow \mathbb{R}^{6 \times 6}\}$ is the compliance matrix; a positive-definite and invertible matrix for regular elasticity (e.g., odd elasticity [51] cannot be covered with this formulation). Note that $\mathbf{S}$ has at most 21 independent parameters [52]. We can now identify

$$\hat{\mathbf{B}}_{\text{elastic}}(\mathbf{x}) = \begin{bmatrix} \rho(\mathbf{x}) \mathbb{1}_{3 \times 3} & \mathbf{0}_{3 \times 6} \\ \mathbf{0}_{6 \times 3} & \mathbf{S} \end{bmatrix}, \quad (17)$$

where $\rho(\mathbf{x})$ denotes the density. To be specific, we further introduce the divergence operator that acts on the stress vector $\text{vec}[\boldsymbol{\sigma}]$ as

$$\mathcal{D} = \begin{bmatrix} \partial_x & 0 & 0 & \partial_y & \partial_z & 0 \\ 0 & \partial_y & 0 & \partial_x & 0 & \partial_z \\ 0 & 0 & \partial_z & 0 & \partial_x & \partial_y \end{bmatrix}. \quad (18)$$

With these definitions, we can find

$$\hat{\mathbf{A}}_{\text{elastic}} = \begin{bmatrix} \mathbf{0}_{3 \times 6} & \mathcal{D} \\ \mathcal{D}^T & \mathbf{0}_{6 \times 3} \end{bmatrix}. \quad (19)$$

Note that $\hat{\mathbf{A}}$ appears symmetric, but it is not: Integration by parts, which shifts the derivative in the inner product, introduces a minus sign, implying that $(\hat{\mathbf{A}}\hat{\mathbf{w}}|\hat{\mathbf{w}}') = -(\hat{\mathbf{w}}|\hat{\mathbf{A}}\hat{\mathbf{w}}')$. The elastic energy is computed as [53]

$$\begin{aligned} (\hat{\mathbf{w}}|\hat{\mathbf{w}})_{\hat{\mathbf{B}}} &= \int_{\Omega} \langle \hat{\mathbf{v}}(\mathbf{x}, t) | \hat{\mathbf{v}}(\mathbf{x}, t) \rangle \rho(\mathbf{x}) d\mathbf{x} \\ &\quad + \int_{\Omega} \langle \hat{\boldsymbol{\sigma}}(\mathbf{x}, t) | \mathbf{S}(\mathbf{x}) | \hat{\boldsymbol{\sigma}}(\mathbf{x}, t) \rangle d\mathbf{x} \\ &= 2E_{\text{kinetic}}(t) + 2E_{\text{potential}}(t). \end{aligned} \quad (20)$$

D. Numerical discretization and boundary conditions

Our framework is compatible with any discretization method, provided that the (anti-)Hermitian properties of the operators are preserved. We represent the numerical discretization of the wave field and operators to vectors and matrices as $\hat{\mathbf{w}} \rightarrow \mathbf{w}$, $\hat{\mathbf{H}} \rightarrow \mathbf{H}$, $\hat{\mathbf{B}} \rightarrow \mathbf{B}$, and $\hat{\mathbf{A}} \rightarrow \mathbf{A}$, where $\mathbf{w} \in \mathbb{R}^L$. The discretized equations of motion read

$$\begin{aligned} \frac{d\mathbf{w}_Q(t)}{dt} &= -i\mathbf{H}\mathbf{w}_Q(t) = \mathbf{B}^{-1/2}\mathbf{A}\mathbf{B}^{-1/2}\mathbf{w}_Q(t), \\ \mathbf{w}_Q(0) &= \mathbf{B}^{1/2}\mathbf{w}_0, \end{aligned} \quad (21)$$

where $\mathbf{A}$ and $\mathbf{B}$ incorporate the BC (Appendix C3).

Preserving the symmetry properties of these operators when discretizing requires that $\mathbf{B}$ is a Hermitian matrix and $\mathbf{A}$ an anti-Hermitian matrix. In Appendix C, we exemplify the symmetry-preserving discretization of the acoustic wave equation using finite differences with a staggered grid [54]. In the context of Maxwell's equations, this choice not only enforces the discrete antisymmetry but also guarantees that Gauss's law remains satisfied for all time [55,56].

In Appendix C, we further show that this discretization naturally gives Neumann or Dirichlet BC on a rectangular domain. Then, starting from the discretization of these particular BCs that respect the symmetries, we discuss in Appendix D

how one can introduce a general class of BC that can be mapped to linear constraints [57]. This includes homogeneous or inhomogeneous Dirichlet or Neumann BC along nonrectangular domain boundaries.

Additionally, $\mathbf{B}$ must be a diagonal or block-diagonal matrix, with block sizes that are independent of the overall system size; otherwise, $\mathbf{B}^{1/2}$ becomes dense and the initial quantum state $\mathbf{w}_Q(0)$ will lack sparsity.

III. RUNTIME ADVANTAGE

Given that the discretized Hamiltonian $\mathbf{H}$ (8) has at most $d = O(1)$ nonzero values in each row and column, which is ensured when $\mathbf{A}$ and $\mathbf{B}$ are d -sparse matrices, and if neither the bit precision m nor the error ϵ is dominating, quantum simulation requires $O(nT) = O(\log NT)$ operations (Theorem 1). This can, in principle, offer an exponential speedup over classical solvers with runtime $O(NT)$ [58–62]. We now show that for the most widely used time-domain classical solvers, we can also establish a runtime lower bound that implies the quantum advantage.

Let us assume black-box, though bounded magnitude, initial conditions and material parameters. Then, for a consistent, causal, and time-local scheme that discretizes the wave equation in both space and time, it is necessary to sample at least at the Nyquist rate $\Delta t \leq 1/(2f_{\max})$, defined by the maximum frequency $f_{\max}$ over all time and space. Only under this condition can the error stay small in the full domain and across all frequencies [63]. Choosing a step that undersamples the wave's period will yield a nonphysical, aliased, or overly smoothed solution. As a result, the scheme must take $\Theta(\frac{T}{\Delta t}) = \Theta(T)$ time steps, updating all N degrees of freedom (DOFs) each step. Consequently, the computational complexity of obtaining a fixed-accuracy solution is lower bounded by $\Omega(NT)$. This applies to all consistent and causal explicit and implicit time integrators.

For example, explicit solvers [64–66] evaluate N d -sparse vector-vector products at each time step. Similarly, implicit solvers [67] require solving a linear system at every time step. Using, for instance, conjugate gradient solvers, this would again require N d -sparse vector-vector products for every step.

However, as we now show, the quantum speedup we can obtain in practice compared to classical solvers is only polynomial [36]. In wave propagation problems, increasing grid points typically aims to (1) enlarge the physical domain or (2) increase the simulated frequencies. For systems with local couplings, such as those resulting from discretizing the considered wave equations, enlarging the domain requires a longer simulation time t for waves to reach the boundaries. Similarly, a finer discretization to simulate higher frequencies raises $\|\mathbf{H}\|_{\max}$ due to the reduced grid spacing. As per Theorem 1, the number of query calls to $\mathcal{H}$ scales linearly with both T and $\|\mathbf{H}\|_{\max}$. Consequently, the quantum speedup over classical algorithms becomes a polynomial factor dependent on the spatial dimension D . Specifically, let $T = \Theta(N^{1/D})$ represent the simulation time for the signal to reach the domain boundary in D dimensions. For classical algorithms scaling linearly with N , the overall runtime complexity is $O(NT) = O(N^{1+1/D})$. In contrast, the HS algorithm has runtime $\tilde{O}(T) =$

$\tilde{O}(N^{1/D})$, where the tilde hides logarithmic factors. Thus, we expect a quadratic speedup in 1D, cubic in 2D, and quartic in 3D. In contrast, Ref. [36] demonstrates an exponential speedup for oscillator models with purely nonlocal couplings, where the simulation time does not scale with the system size.

One fundamental requirement for any quantum advantage compared to classical solvers is that the oracle $\mathcal{H}$ can be implemented efficiently. To address this, let us first separate $\mathcal{H}$ into an oracle $\mathcal{A}$ that implements $\mathbf{A}$ and an oracle $\mathcal{B}^{-1/2}$ that implements $\mathbf{B}^{-1/2}$. If we have access to both $\mathcal{A}$ and $\mathcal{B}^{-1/2}$, we can always efficiently implement $\mathcal{H}$ based on Eq. (21) and the multiplication property of block encodings [68]. Hence, it suffices to show that both have efficient circuit implementations.

The matrix $\mathbf{A}$ can be efficiently constructed using the finite-difference method [68–71]. The material matrix $\mathbf{B}$, however, poses information-theoretical limitations, even for the simplest case where $\mathbf{B}$ is diagonal. In this case, $\mathbf{B}^{-1/2}$ inherits the diagonality and we can directly parameterize $\mathbf{B}^{-1/2}$ as a linear combination of diagonal unitary basis functions with the linear-combination-of-unitaries technique [26]. It has been shown that certain diagonal unitary matrices have efficient circuit implementations [72]. However, even if each individual unitary matrix can be implemented efficiently, the number of unitaries must still be bounded. This gives rise to a general information-theoretical limitation: To preserve quantum speedup, within the query model the information transferred to the QC must be of order $O(\text{polylog}(N))$ for each query. This limits the number of independent material parameters that define $\mathbf{B}^{-1/2}$ to this order, necessitating functional or low-dimensional material representations. To illustrate, let us consider a model that is described by $O(N)$ bits of information. Let us furthermore assume that either (1) this information is incompressible or (2) a compression can only be found in $\Omega(N)$. This assumption is generally valid, as the compression of a linear system reduces to an NP-complete subset selection problem [73]. All of this information needs to be loaded to the quantum computer, which takes $O(N)$ initialization operations under the standard circuit-based encoding model. This dominates the runtime of the forward model and prevents all runtime advantages. We expect that low-dimensional material representations can exist for media characterized by a sufficiently small set of basis functions or for random media [74] that are characterized by limited information such as the mean and variance of the distribution.

IV. ESTIMATING SUBSPACE l_2 NORMS AND ENERGIES

Reading the complete discrete wave field $\mathbf{w}_Q(t)$ from a quantum state comes with exponential and, hence, prohibitive costs. Consequently, it is essential to perform computations with the simulated wave field directly on the QC, e.g., by evaluating loss functions. We show that it is possible to efficiently measure l_2 norms of state subspaces containing multiple superposed quantum states, and that this measurement achieves optimal precision scaling with the number of experiment evaluations:

Theorem 2 (Subspace l_2 norm, Appendix A 2). Let $\{\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_M\} \in \mathbb{C}^L$. Given a projector $\mathbf{P}_S = \text{diag}(p_1, p_2, \dots, p_L)$, which projects onto a subspace $S \subseteq \mathbb{C}^L$, where each $p_i \in \{0, 1\}$ and $d = \sum_{i=1}^L p_i$. Let there

be a state preparation oracle $\mathcal{U}$ that prepares the quantum state $|\phi\rangle = [\mathbf{w}_1; \mathbf{w}_2; \dots; \mathbf{w}_M]/\|[\mathbf{w}_1; \mathbf{w}_2; \dots; \mathbf{w}_M]\|$. Then, if either $d = O(\text{polylog}(L))$ or $L - d = O(\text{polylog}(L))$, there exists a quantum algorithm that efficiently estimates the squared sum of $\{\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_M\}$ on $\mathcal{S}$ as

$$l_S^2 = \|\mathbf{P}_S \mathbf{w}_1 + \mathbf{P}_S \mathbf{w}_2 + \dots + \mathbf{P}_S \mathbf{w}_M\|^2, \quad (22)$$

with probability at least $1 - \delta$ within error ϵ , which makes $O(M \log(1/\delta)/\epsilon)$ calls to the oracle $\mathcal{U}$ (along with its inverse and controlled versions).

We will now apply this result to compare two wave fields such as a simulated and a target $\mathbf{B}^{1/2}$ -transformed wave field and to measure subvolume energies (see Sec. II). By setting $M = 2$, $\mathbf{w}_1 = \mathbf{w}_Q$, $\mathbf{w}_2 = -\mathbf{w}_Q^{\text{target}}$, where $\mathbf{w}_Q$ is the simulated wave field and $\mathbf{w}_Q^{\text{target}}$ is a target or observed wave field that is only defined or known within subvolume $\mathcal{S}$, we can write

$$l_S^2 = \|\mathbf{P}_S \mathbf{w}_Q - \mathbf{P}_S \mathbf{w}_Q^{\text{target}}\|^2. \quad (23)$$

This corresponds to an estimate of the l_2 distance between both fields on subspace $\mathcal{S}$. By setting $M = 1$, $\mathbf{w}_1 = \mathbf{w}_Q$, we obtain

$$l_S^2 = \|\mathbf{P}_S \mathbf{w}_Q\|^2, \quad (24)$$

which estimates the energy of $\mathbf{w}$ on $\mathcal{S}$. Theorem 2 can also be used to compute energies and l_2 comparisons of a superposition of multiple wave fields, extending the work of Ref. [36] on measuring energies. These multistate l_2 and energy estimates are key components of the source implementation algorithm, which we will introduce in Sec. V.

We can utilize a weighted inner product to compare states in the standard, non- $\mathbf{B}^{1/2}$ -transformed bases, as detailed in Appendix A 3. However, as we discuss in Sec. VIA, this will result in globality issues in general. In practice, e.g., within the domain of inverse problems, it is usually sufficient to compare transformed wave fields.

Finally, given an efficient quantum algorithm for a unitary basis transformation, comparisons can also be performed in bases other than the computational basis. This, for example, includes the spatial frequency domain, which can be efficiently accessed through the quantum Fourier transform [22].

V. IMPLEMENTING SOURCES

Incorporating time-dependent sources into the HS of classical wave equations poses a significant challenge when aiming to maintain efficient runtime scaling, as in this framework the wave evolution is unitary and, hence, inherently source free. We consider a source term that is constituted of S sources,

$$\hat{\mathbf{s}}(\mathbf{x}, t) = \sum_{s=1}^S \chi_s(\mathbf{x}) f_s(t), \quad (25)$$

where $\chi_s \in \mathbb{R}^D \rightarrow \mathbb{R}^C$ is the spatial distribution of the s th sources and $f_s(t)$ is its source-time function.

Assuming that χ_s is a point source and f_s is a pulse function, whose support in time is compact and with a length either constant or inversely proportional to the maximum frequency, we will show that we can classically map the source to sparse initial conditions with an implementation complexity

of $O(1)$. This already covers many practically relevant source scenarios. We then show how to implement sources that lack compact support in time, but that give rise to rotationally covariant wave fields.

A. Single pulse source

Consider a single point source defined by

$$\hat{\mathbf{s}}(\mathbf{x}, t) = \hat{\chi} \delta(\mathbf{x} - \mathbf{x}_s) f(t), \quad (26)$$

where $\hat{\chi} \in \mathbb{R}^C$ is an arbitrary vector. Its implementation complexity is tied to the number of values that need to be initialized on the QC. We identify two optimal scenarios:

1. Fixed source duration

If the simulation domain grows while the source remains active over a fixed duration $\Delta T = T^{\text{end}} - T^{\text{start}}$, the implementation complexity naturally stays $O(1)$. This is achieved by

(1) classically solving the forced wave equation over ΔT within a fixed volume around the source, sufficient to contain all emitted waves during this interval;

(2) initializing the resulting sparse wave field on the QC.

Since the required initialization volume does not scale with N , only a constant number of grid points needs to be initialized, ensuring $O(1)$ runtime complexity.

2. Increasing grid resolution

When refining the grid to simulate higher-frequency wave pulses, typically the source-time function $f(t)$ includes higher frequencies, resulting in a duration inversely proportional to the increased frequency bandwidth $\Delta\omega$:

$$\Delta T \propto \frac{1}{\Delta\omega} = \frac{1}{\omega^{\text{max}} - \omega^{\text{min}}}, \quad (27)$$

where $[\omega^{\text{min}}, \omega^{\text{max}}]$ is the support of the Fourier transform $\tilde{f}(\omega)$ of $f(t)$. For example, increasing the grid resolution by a factor of 2 (i.e., halving the spatial grid spacing $\Delta x \rightarrow \Delta x/2$) allows us to resolve higher spatial frequencies. If we scale the frequency bounds of $f(t)$ as $\omega^{\text{max}} \rightarrow 2\omega^{\text{max}}$ and $\omega^{\text{min}} \rightarrow \alpha \omega^{\text{min}}$ with $\alpha \leq 2$, then this results in at least a doubling of $\Delta\omega$ and thus halving ΔT . Consequently, the classically simulated volume decreases proportionally across all dimensions, and the number of initialized grid points remains constant, maintaining $O(1)$ complexity.

B. Multiple pulse sources

We extend our analysis to sources composed of multiple point sources:

$$\hat{\mathbf{s}}(\mathbf{x}, t) = \sum_{s=1}^S \hat{\chi}_s \delta(\mathbf{x} - \mathbf{x}_s) f_s(t). \quad (28)$$

1. Synchronous activation

If all sources are active over the same time interval, i.e., $T_s^{\text{start}} = T^{\text{start}}$ and $T_s^{\text{end}} = T^{\text{end}}$ for all s , the previous approach applies directly. Each source can be classically simulated within its respective volume, and the resulting wave fields are

initialized on the QC as a single initial condition. The runtime scaling remains $O(1)$ provided that the number of sources S does not scale with N .

2. Asynchronous activation

When activation times vary among different point sources, an additional step is required to synchronize them. Let $\mathbf{w}_s$ for $s = 1, \dots, S$ denote the initial conditions from classically simulating each source over their respective durations $\Delta T_s = T_s^{\text{end}} - T_s^{\text{start}}$. The combined and energy-transformed initial state is given by

$$\phi(0) = (I^{\otimes \log_2(S)} \otimes \mathbf{B}^{1/2})[\mathbf{w}_1; \dots; \mathbf{w}_S], \quad (29)$$

where

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (30)$$

The initial quantum state then is

$$|\psi(0)\rangle = \frac{\phi(0)}{\|\phi(0)\|}, \quad (31)$$

incorporating initial conditions at different global times. To synchronize these states to a common global time $T^{\text{sync}} = \max\{T_1^{\text{end}}, \dots, T_S^{\text{end}}\}$, we evolve the state using a time-dilating Hamiltonian $\mathbf{H}^{\text{sync}}$:

$$|\psi(T^{\text{sync}})\rangle = e^{-i\mathbf{H}^{\text{sync}}} |\psi(0)\rangle, \quad (32)$$

where

$$\mathbf{H}^{\text{sync}} = \begin{bmatrix} (T^{\text{sync}} - T_1^{\text{end}})\mathbf{H} & \dots & \mathbf{0} \\ \vdots & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & (T^{\text{sync}} - T_S^{\text{end}})\mathbf{H} \end{bmatrix}. \quad (33)$$

This effectively time-dilates each component, aligning them to T^{sync} . Subsequently, the synchronized state is evolved under the multistate wave equation Hamiltonian $\mathbf{H}^{\text{mult}} = I^{\otimes \log_2(S)} \otimes \mathbf{H}$ to the final simulation time T :

$$|\psi(T)\rangle = e^{-i(T - T^{\text{sync}})\mathbf{H}^{\text{mult}}} |\psi(T^{\text{sync}})\rangle. \quad (34)$$

Due to the linearity of the wave equation, the superposition of partial wave fields in $|\psi(T)\rangle$ corresponds to the solution of Eq. (21) at time T . Consequently, we can estimate an l_2 distance to a target field or subspace energies using Theorem 2. Since the addition operation is inherently nonunitary, it must be integrated within the measurement process. Furthermore, as the loss function is nonlinear, we cannot compute losses for individual subfields separately and then combine them classically to derive the joint loss; therefore, we have to rely on Theorem 2 to estimate the loss function.

This approach remains efficient under the conditions that (1) the number of point sources S is independent of N and (2) each individual source meets the previously outlined constraints.

C. Rotationally symmetric sources without compact support in time

Implementing a source-time function $f(t)$ that lacks compact support in time is inefficient with the above approach, as it results in initial conditions lacking compact support in

space. Such initial fields are prohibitively expensive to compute classically and initialize on the QC.

To target this, we introduce an algorithm that efficiently initializes rotationally covariant wave fields as quantum states:

Lemma 1 (Vector Field Initialization, Appendix B 1). Let $\mathbf{w}^{\text{sym}} : \mathbb{R}^D \rightarrow \mathbb{R}^C$ be a vector field. Assume that $\mathbf{w}^{\text{sym}}$ is rotationally covariant around a point $\mathbf{x}_0 \in \mathbb{R}^D$. Consider an isotropic radially symmetric grid centered at $\mathbf{x}_0$, discretized into $N = A^D$ points, where A is the number of radial divisions. The grid points are specified by radial indices $a \in \{1, \dots, A\}$ and angular indices θ . Define the quantum state

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{c=1}^C \sum_{a=1}^A \sum_{\theta} w_c^{\text{sym}}(\mathbf{x}_{a,\theta}) |c\rangle \otimes |a\rangle \otimes |\theta\rangle, \quad (35)$$

where $w_c^{\text{sym}}(\mathbf{x}_{a,\theta})$ is the c th component of $\mathbf{w}^{\text{sym}}$ at grid point $\mathbf{x}_{a,\theta}$, and $\mathcal{N} = \sum_{c,a,\theta} |w_c^{\text{sym}}(\mathbf{x}_{a,\theta})|^2$ ensures normalization. This state can be initialized with $O(N^{1/D})$ classical evaluations of $\mathbf{w}^{\text{sym}}$ and $\tilde{O}(CN^{1/D})$ quantum gates, where the tilde hides polylogarithmic factors.

We consider a spatial source distribution $\chi = \chi^{\text{sym}}$ for which an arbitrary rotation in space and the same rotation of the source vector yield the same result. Formally, let there be a $\mathbf{R}(\mathbf{S}) \in \text{SO}(C)$, where $\mathbf{S} \in \text{SO}(D)$; then, rotationally covariant sources satisfy $\mathbf{R}(\mathbf{S})\chi^{\text{sym}}(\mathbf{x}) = \chi^{\text{sym}}(\mathbf{S}\mathbf{x}) \forall \mathbf{x}, \mathbf{S}$. We further denote the rotationally covariant Green's function that solves wave Eq. (1) in a homogeneous medium for the source $\hat{\mathbf{s}}_\delta(\mathbf{x}, t) = \chi^{\text{sym}}(\mathbf{x})\delta(t)$ as $\hat{\mathbf{G}}^{\text{sym}}$. In this case, the wave field arising from the source-time function f is given by $\hat{\mathbf{w}}^{\text{sym}} = \hat{\mathbf{G}}^{\text{sym}} * f$. It can be discretized as $\hat{\mathbf{w}}^{\text{sym}} \rightarrow \mathbf{w}^{\text{sym}}$ and efficiently initialized on a spherical grid centered around the source location using Lemma 1.

Now let us assume that the medium is generally heterogeneous but there exists a small homogeneous volume around the source with radius r_s . This may hold true in certain experimental setups and can otherwise be taken as an approximation. Let the travel time in the volume be $T_s^{\text{hom}} = r_s/c^{\text{hom}}$, where c^{hom} is the wave speed in the homogeneous medium. If the source-time function is active for time period $T_s > T_s^{\text{hom}}$, then we can split the source in $J \approx T_s/T_s^{\text{hom}}$ contributions:

$$f(t) \approx \sum_{j=1}^J W_j(t - \tau_j) f(t), \quad (36)$$

where W_j are sigmoid window functions (see Appendix B 2 for details). All J source terms for $f(t)$ can be recognized as individual sources that satisfy $\Delta T_j \leq T_j^{\text{hom}}$, where ΔT_j is the duration of the j th source. This means that for none of them, the corresponding wave leaves the homogeneous domain before it terminates. Therefore, the resulting J initial wave fields are all rotationally covariant:

$$\hat{\mathbf{w}}_j^{\text{sym}}(\mathbf{x}, t - \tau_j) = \hat{\mathbf{G}}^{\text{sym}}(\mathbf{x}, t) * (W_j(t) f(t + \tau_j)), \\ \times |\mathbf{x}| < r, \quad j = 1, \dots, J. \quad (37)$$

By using the same discretization as in the homogeneous case, we can initialize the state $[\mathbf{w}_1^{\text{sym}}; \dots; \mathbf{w}_J^{\text{sym}}]$ with a runtime complexity of $\tilde{O}(JCN^{1/D})$. This state can then be synchronized and measured as introduced in Sec. VB 2. Hence, if

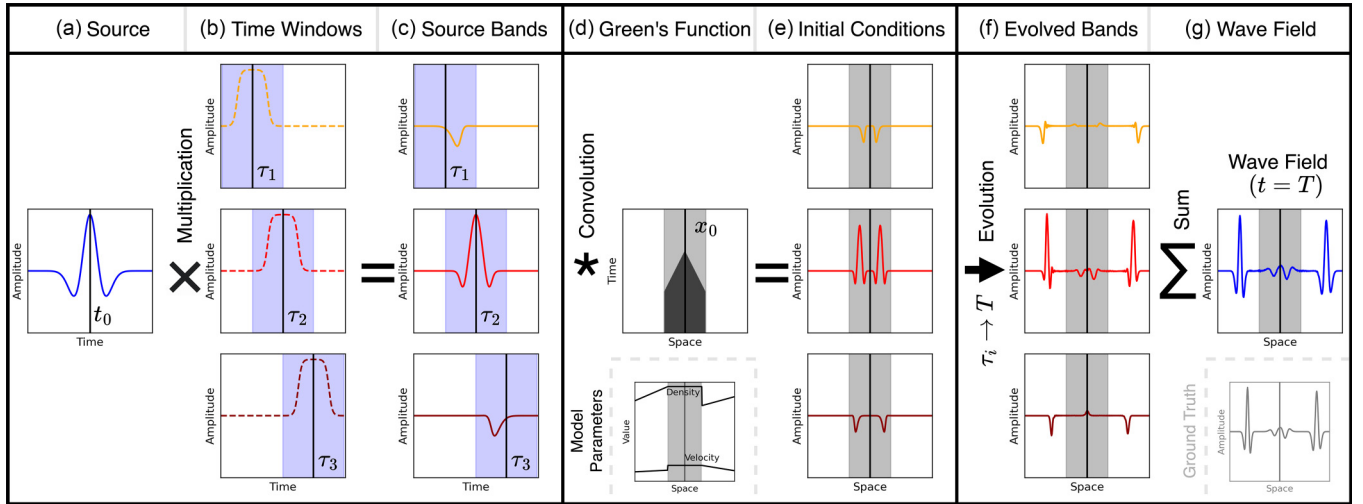


FIG. 1. Algorithm implementing a point source function on a QC for a 1D acoustic problem. Panel (a) shows the source-time function for a single point location. We decompose the source-time function in time (b), which gives a set of functions that, in superposition, equate to the original source-time function (c). The inset at the bottom shows the acoustic parameters' profiles with the homogeneous volume around the source. By convolving them in time with the homogeneous Green's function (d), we obtain multiple sets of initial conditions at different global times (e). We evolve these initial conditions over different time intervals to the final simulation time T (f). Here, the superposition of the source slices is equal to the solution of the wave equation (g). We can utilize this to efficiently estimate an l_2 distance to a target state using Theorem 2.

$J = \tilde{O}(\text{polylog}(N))$, the runtime advantage remains. The whole workflow is depicted in Fig. 1.

Note that the rotationally covariant initial wave field must be precomputed classically along a reference direction on the spherical grid with a runtime complexity of at worst $\tilde{O}(CN^{1/D})$. This is, for example, possible via analytic Green's functions for acoustic and elastic isotropic (explosive) point sources.

Finally, the complexity scales linearly with the number of sources. Therefore, the number of sources must not scale worse than $\text{polylog}(N)$ to preserve the overall speedup.

VI. LIMITATIONS

The limitations considered here are those that either impact the algorithmic runtime in terms of big- O complexity or are fundamentally not implementable in this framework.

A. Loss functions

We identify two limitations within the loss function estimations introduced:

(1) Estimating time-integrated loss functions: Currently, our algorithm estimates the loss at a single measurement time step. Computing time-integrated loss functions involves separate simulation experiments for each measurement time, with the overall loss metric computed across all steps using either Theorem 2 or classical postprocessing. However, this approach becomes inefficient for long comparison/integration times, where the number of comparison time steps scales worse than $O(\text{polylog}(N))$. Nondestructive estimation of the loss function [75,76] could provide a solution by preserving the state throughout the measurement operation, enabling iterative evolution and loss estimation of the wave field for multiple time points.

(2) Globality of measurement quantities: A limitation of QC loss estimation via observable measurements is the requirement for sufficiently global measurement quantities. Suppose a state is measured in a subspace with only a small probability amplitude fraction compared to the entire quantum state. In that case, more samples are needed to estimate the norm accurately, as the expected value becomes vanishingly small. For example, ensuring the subspace size is large with respect to N can mitigate this issue in practice.

B. Source terms

We identify four limitations:

(1) The number of sources in space must not scale worse than $O(\text{polylog}(N))$. For instance, it is inefficient to have a source everywhere on the surface of a 3D body.

(2) Situations where the number of initialized nonzero values grows polynomially with N must be avoided to prevent restricting the overall runtime. An example of this could be a continuously active source within an inhomogeneous medium.

(3) For symmetric sources without compact time support, the requirement for radially symmetric grids may be practically limiting as domains can be nonsymmetric around the source location.

(4) Finally, for sources without compact spatial support in a generally inhomogeneous medium, or for nonrotationally covariant sources, the runtime advantage is lost because the resulting wave field lacks symmetry, and Lemma 1 can no longer be employed.

C. Damping

Damping in the context of HS has been recently studied, demonstrating that quantum speedup can be preserved under

certain conditions [77,78]. An alternative approach is to map a damped classical wave equation to an open quantum system [79], or to represent nonunitary time evolution as a linear combination of unitary operations [80,81]. The latter approach appears particularly well suited to our framework and is the focus of an ongoing follow-up study.

D. Time-dependent media

Another remark concerns time-dependent media, such as those in time-modulated metamaterials [82–84]. In these cases, $\mathbf{B} = \mathbf{B}(t)$ becomes time-dependent, implying that it no longer commutes with the time derivative. Consequently, a time-dependent symmetric problem is mapped to a time-dependent non-Hermitian Schrödinger equation, rendering the introduced framework inapplicable [85].

E. Hardware

A final limitation of the proposed framework is its reliance on fault-tolerant quantum hardware. While the employed HS algorithm achieves optimal asymptotic runtime in the error-free regime, alternative forward algorithms may perform better on real-world problems in the noisy intermediate-scale quantum regime [86–88]. Investigating the compatibility with near-term hardware and the associated runtime implications is left for future work.

VII. CONCLUSIONS

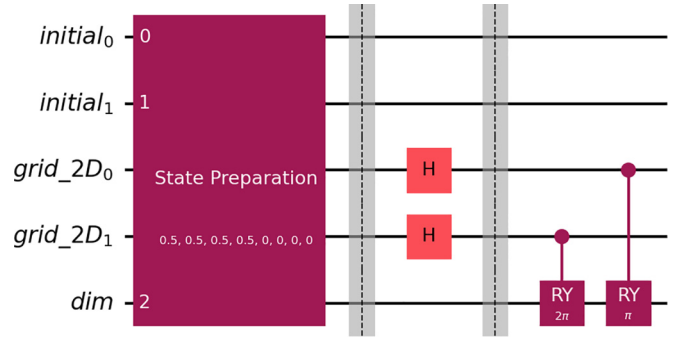
In this work, we have demonstrated that we can efficiently simulate forced, linear, anti-Hermitian wave equations with arbitrary heterogeneous and anisotropic material properties within the HS framework. While the theoretical speedup of this approach can be exponential, practical 3D applications are expected to see a quartic speedup due to the scaling of the simulation time with the system size. This quartic speedup is maintained throughout our algorithm if the state readout is sufficiently global compared to the overall system size.

Our method is compatible with any numerical approach that respects the anti-Hermitian nature of the operator and results in a diagonal or block diagonal representation of the material properties. The introduced representation of the wave equations naturally leads to a quantum encoding that enables the measurement of energies in subvolumes of the model with optimal precision scaling in the number of measurements taken. Additionally, we have shown that the l_2 distance of the final simulated wave field to a target or observed wave field can be measured with optimal precision scaling and that a broad class of source terms can be implemented efficiently.

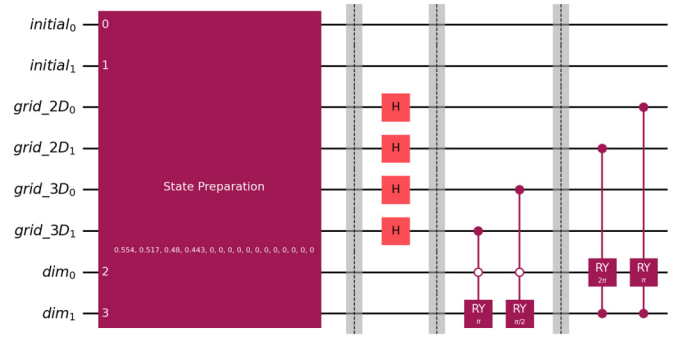
New advances in quantum error correction hint that noise-free QC might be realized soon [89]. These findings suggest that our proposed framework may have practical applications in the near future, thereby underscoring the importance of continued research in this field.

ACKNOWLEDGMENTS

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(a) 2D Initialization circuit. The full vector field is constructed from a single ray in $[1, 0]$ direction.



(b) 3D Initialization circuit. The full vector field is constructed from a single ray in $[1, 0, 0]$ direction.

FIG. 2. Quantum circuits for efficient vector field initialization in 2D and 3D. The initial ray is prepared in the quantum register *initial* with vector components saved in the register *dim*. The register *grid_{2D}* (and *grid_{3D}*) is transformed into a state of equal superposition. Afterward (multi)controlled RY rotations are applied with decreasing angles, which gives the rotationally symmetric vector field in the combined registers.

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Study conception: C.B.; sources: M.S. and C.B.; loss functions and energy estimation: M.S., C.B., and S.K.; acoustic FD implementation: G.A.; general boundary conditions and constraints: G.A. and C.B.; manuscript preparation: M.S., C.B., G.A., S.K., and A.F. All authors reviewed the results and approved the final version of the manuscript.

DATA AVAILABILITY

The data and code that support the findings of this article are openly available [90]. The code includes numerical wave simulations based on the algorithms presented in the article. Additionally, the code generates Fig. 2.

APPENDIX A: ESTIMATING LOSS FUNCTIONS

To prove Theorem 2, we first introduce the following auxiliary result:

Lemma A1 (Two-state subspace l_2 norm, Appendix A 1). Let $\mathbf{a}, \mathbf{b} \in \mathbb{C}^L$. Given a projector $\mathbf{P}_S = \text{diag}(p_1, p_2, \dots, p_L)$, which projects onto a subspace $\mathcal{S} \subseteq \mathbb{C}^L$, where each $p_i \in \{0, 1\}$ and $d = \sum_{i=1}^L p_i$. Let there be a state preparation oracle $\mathcal{U}$ that prepares the quantum state $|\phi\rangle = [\mathbf{a}; \mathbf{b}] / \|\mathbf{a}; \mathbf{b}\|$. Then, if either $d = O(\text{polylog}(L))$ or $L - d = O(\text{polylog}(L))$, there exists a quantum algorithm that efficiently estimates the $l_{2,S}$ norm between $\mathbf{a}$ and $\mathbf{b}$ on $\mathcal{S}$ as

$$l_{2,S}^2 = \|\mathbf{P}_S \mathbf{a} - \mathbf{P}_S \mathbf{b}\|^2, \quad (\text{A1})$$

with probability at least $1 - \delta$ within error ϵ , which makes $O(\log(1/\delta)/\epsilon)$ calls to the oracle $\mathcal{U}$ (along with its inverse and controlled versions).

1. Proof of Lemma A1

The squared l_2 norm on this subspace is defined as

$$l_{2,S}^2 = \sum_i^L |(\mathbf{P}_S \mathbf{a})_i - (\mathbf{P}_S \mathbf{b})_i|^2. \quad (\text{A2})$$

By introducing $|\phi\rangle = [\mathbf{a}; \mathbf{b}] / \|\mathbf{a}; \mathbf{b}\|$, we can write Eq. (A2) as an expected value estimation:

$$l_{2,S}^2 = \langle \phi | \mathbf{O} | \phi \rangle \|\mathbf{a}; \mathbf{b}\|^2, \quad (\text{A3})$$

where the Hermitian observable $\mathbf{O}$ is given by

$$\mathbf{O}_{2L \times 2L} = \begin{bmatrix} \mathbf{P}_S & -\mathbf{P}_S \\ -\mathbf{P}_S & \mathbf{P}_S \end{bmatrix}. \quad (\text{A4})$$

The observable $\mathbf{O}$ can be recognized as a difference operator that estimates the l_2 norm between $\mathbf{a}$ and $\mathbf{b}$ on the subspace $\mathcal{S}$ up to normalization and can, in principle, be implemented on a QC with suboptimal precision scaling [22].

To estimate $l_{2,S}^2$ with optimal precision scaling beyond the central limit, we will introduce an auxiliary qubit to double the state space dimension. In this augmented space, we can find a unitary decomposable observable $\tilde{\mathbf{O}}$, whose expectation value with respect to the augmented state $|\psi\rangle = [\mathbf{P}_S \mathbf{a}; \mathbf{P}_S \mathbf{b}; (\mathbf{1} - \mathbf{P}_S) \mathbf{a}; (\mathbf{1} - \mathbf{P}_S) \mathbf{b}] / \|\mathbf{a}; \mathbf{b}\|$ is equal to $l_{2,S}$, such that

$$l_{2,S}^2 = \langle \psi | \tilde{\mathbf{O}} | \psi \rangle \|\mathbf{a}; \mathbf{b}\|^2. \quad (\text{A5})$$

We first demonstrate that there exists a unitary initialization procedure for $|\psi\rangle$ given an initialization oracle for $|\phi\rangle$ and discuss the efficiency of its implementation. We then explicitly construct $\tilde{\mathbf{O}}$, which can be decomposed into four commuting unitary observables independent of L and $\mathcal{S}$. We conclude by analyzing the overall complexity of our algorithm.

To start, let us combine $\mathbf{U}_a$ preparing $\mathbf{a}$ and $\mathbf{U}_b$ preparing $\mathbf{b}$ into a single unitary $\mathbf{U}$ that prepares $|\phi\rangle$ as

$$|\phi\rangle = \mathbf{U} |0^{n+1}\rangle = \begin{bmatrix} \mathbf{U}_a & 0 \\ 0 & \mathbf{U}_b \end{bmatrix} |0^{n+1}\rangle, \quad (\text{A6})$$

where $n = \log_2(L)$. We further define the unitary matrix $\tilde{\mathbf{P}}_S \in \mathbb{C}^{4L \times 4L}$ constructed from $\mathbf{P}_S$ and its complement subspace $\mathbf{1} - \mathbf{P}_S$ as

$$\tilde{\mathbf{P}}_S = \begin{bmatrix} \mathbf{P}_S & 0 & (\mathbf{1} - \mathbf{P}_S) & 0 \\ 0 & \mathbf{P}_S & 0 & (\mathbf{1} - \mathbf{P}_S) \\ (\mathbf{1} - \mathbf{P}_S) & 0 & \mathbf{P}_S & 0 \\ 0 & (\mathbf{1} - \mathbf{P}_S) & 0 & \mathbf{P}_S \end{bmatrix}. \quad (\text{A7})$$

By adding one auxiliary qubit, which is left invariant during the application of $\mathbf{U}$, the target state $|\psi\rangle$ can finally be obtained as

$$|\psi\rangle = \tilde{\mathbf{P}}_S (I \otimes \mathbf{U}) |0^{n+1}\rangle = [\mathbf{P}_S \mathbf{a}; \mathbf{P}_S \mathbf{b}; (\mathbf{1} - \mathbf{P}_S) \mathbf{a}; (\mathbf{1} - \mathbf{P}_S) \mathbf{b}] / \|\mathbf{a}; \mathbf{b}\|, \quad (\text{A8})$$

where

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (\text{A9})$$

As $\mathbf{P}_S$ is diagonal, $\tilde{\mathbf{P}}_S$ can be recognized as a permutation matrix, which is decomposable into $\tilde{\mathbf{P}}_S = \prod_j^d \tilde{\mathbf{P}}_{S_j}$. Each $\tilde{\mathbf{P}}_{S_j}$ can be implemented with one multicontrolled X gate (MCX). As MCX gates can be synthesized with $O(n)$ controlled-not gates with a circuit depth of $O(\log_2(n))$ using $O(n)$ auxiliary qubits [91–93], the overall gate complexity when implementing $\tilde{\mathbf{P}}_S$ is $O(dn)$ with a circuit depth of $O(d \log_2(n))$. Hence, if either $d = O(\text{polylog}(L))$ or $L - d = O(\text{polylog}(L))$, the implementation of $\tilde{\mathbf{P}}_S$ is guaranteed to be efficient.

As future QC might allow for implementing hardware native MCX gates, further reductions in gate complexity are possible [94–96]. Additionally, regular patterns in $\tilde{\mathbf{P}}_S$ can be exploited to implement multiple $\tilde{\mathbf{P}}_{S_j}$ at once. Even for large d , this can allow for an efficient implementation of $\tilde{\mathbf{P}}_S$ in some instances, e.g., for projections to the first half of the domain.

We now introduce the augmented observable

$$\tilde{\mathbf{O}}_{4L \times 4L} = \begin{bmatrix} \mathbf{1} & -\mathbf{1} & 0 & 0 \\ -\mathbf{1} & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (\text{A10})$$

Using the definition of $|\psi\rangle$, it is easy to check that

$$l_{2,S}^2 = \langle \psi | \tilde{\mathbf{O}} | \psi \rangle \|\mathbf{a}; \mathbf{b}\|^2. \quad (\text{A11})$$

The augmented observable $\tilde{\mathbf{O}}$ is always—independent of the state dimension L and the subspace $\mathcal{S}$ —represented by the four Pauli matrices

$$\begin{aligned} \tilde{\mathbf{O}}_1 &= I \otimes I \otimes I \otimes \dots \otimes I, \\ \tilde{\mathbf{O}}_2 &= I \otimes X \otimes I \otimes \dots \otimes I, \\ \tilde{\mathbf{O}}_3 &= Z \otimes I \otimes I \otimes \dots \otimes I, \\ \tilde{\mathbf{O}}_4 &= Z \otimes X \otimes I \otimes \dots \otimes I, \end{aligned} \quad (\text{A12})$$

where

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (\text{A13})$$

and with coefficients $\mathbf{c} = [0.5, -0.5, 0.5, -0.5]$, such that

$$\tilde{\mathbf{O}} = \sum_{j=1}^4 \mathbf{c}_j \tilde{\mathbf{O}}_j. \quad (\text{A14})$$

Hence, we conclude that $l_{2,S}^2$ can be estimated as

$$l_{2,S}^2 = \|\mathbf{a}; \mathbf{b}\|^2 \sum_{j=1}^4 \mathbf{c}_j \langle \psi | \tilde{\mathbf{O}}_j | \psi \rangle. \quad (\text{A15})$$

As proven in Ref. [97], the measurement of the expected value of a quantum state with respect to an observable that is unitary using high-fidelity amplitude amplification techniques has optimal precision scaling with a query complexity of $O(\log(1/\delta)/\epsilon)$. As all Pauli observables are unitary and the number of Pauli observables that represent $\tilde{\mathbf{O}}$ is independent of L and S , it follows that our algorithm has the same query complexity.

2. Proof of Theorem 2

Building on Lemma A1, we can estimate general l_2 norms of arbitrary many substates. Consider a quantum state

$$|\phi\rangle = [\mathbf{w}_1; \mathbf{w}_2; \dots; \mathbf{w}_M] / \|\mathbf{w}_1; \mathbf{w}_2; \dots; \mathbf{w}_M\|, \quad (\text{A16})$$

with $\mathbf{w}_i \in \mathbb{C}^L$, where M is the number of substates. We aim to estimate a squared l_2 norm l_{Σ}^2 on a subspace S defined by the projector $\mathbf{P}_S$, such that

$$l_{\Sigma,S}^2 = \|\mathbf{P}_S \mathbf{w}_1 + \mathbf{P}_S \mathbf{w}_2 + \dots + \mathbf{P}_S \mathbf{w}_M\|^2. \quad (\text{A17})$$

It remains to generalize $\tilde{\mathbf{P}}_S$ [see Eq. (A7)] and $\tilde{\mathbf{O}}$ [see Eq. (A14)].

We extend $\tilde{\mathbf{P}}_S$ by recognizing that it corresponds to the unitary matrix:

$$\tilde{\mathbf{P}}_{S,A} = \begin{bmatrix} \mathbf{P}_S & (\mathbb{1} - \mathbf{P}_S) \\ (\mathbb{1} - \mathbf{P}_S) & \mathbf{P}_S \end{bmatrix}, \quad (\text{A18})$$

which is then tensor-multiplied with a number of I gates depending on M , such that

$$\tilde{\mathbf{P}}_{S,\Sigma} = \tilde{\mathbf{P}}_{S,A} \otimes I^{\otimes \log_2(M)}. \quad (\text{A19})$$

Similarly, the specific structure of $\tilde{\mathbf{O}}$ lets us define the generalized observable $\tilde{\mathbf{O}}_{\Sigma}$ as

$$\tilde{\mathbf{O}}_{\Sigma} = \frac{1}{2}(I \otimes \tilde{\mathbf{O}}_A + Z \otimes \tilde{\mathbf{O}}_A) \otimes I^{\otimes \log_2(L)}, \quad (\text{A20})$$

where

$$\tilde{\mathbf{O}}_A = \sum_{\mathbf{A} \in \{I, X\}^{\otimes \log_2(M)}} \mathbf{A}. \quad (\text{A21})$$

In this context, Eq. (A20) represents the half-domain measurement of $|\psi\rangle$ through

$$\frac{1}{2}(I + Z) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad (\text{A22})$$

and the dimension of each substate $\mathbf{w}_i$ as $\dim(I^{\otimes \log_2(L)}) = L \times L$, while Eq. (A21) describes the summation of the substates.

The number of Pauli observables in Eq. (A21) depends on M , as $|\{I, X\}^{\otimes \log_2(M)}| = M$. Therefore, the number of unitary observables that need to be estimated is $2M$. Consequently, the overall query complexity of the algorithm is $O(M \log(1/\delta)/\epsilon)$. For verification, with $M = 2$, $\mathbf{w}_1 = \mathbf{a}$, and $\mathbf{w}_2 = -\mathbf{b}$, we see that $\tilde{\mathbf{O}}_{\Sigma} = \tilde{\mathbf{O}}$ and $\tilde{\mathbf{P}}_{S,\Sigma} = \tilde{\mathbf{P}}_S$, confirming that $l_{\Sigma,S}^2 = l_{2,S}^2$.

3. Weighted l_2 norms

To compare the states in the standard basis, we utilize a weighted inner product that reverses the transformation with $\mathbf{B}^{1/2}$:

Corollary A1 (Weighted l_2 norm). Given Theorem 2, we can estimate a weighted l_2 norm with $O(V \log(1/\delta)/\epsilon)$ calls to the oracle $\mathcal{U}$ (along with its inverse and controlled versions), as

$$l_v^2 = \sum_j^V v_j l_{S_j}^2, \quad (\text{A23})$$

where $\mathbf{v} \in \mathbb{R}_+^V$ is a weight vector consisting of all V unique weights. The estimation is efficient if the number of unique weights satisfies $V = O(\text{polylog}(L))$, and if for every $\mathbf{P}_{S_j}$ either $d_j = O(\text{polylog}(L))$ or $L - d_j = O(\text{polylog}(L))$.

Applying this to the comparison between two wave fields, we obtain

$$\begin{aligned} l_B^2 &= \sum_j^{\bar{B}} B_j^{-1/2} \|\mathbf{P}_{S_j} \mathbf{w}_Q - \mathbf{P}_{S_j} \mathbf{w}_Q^{\text{target}}\|^2 \\ &= \sum_j^{\bar{B}} \|\mathbf{P}_{S_j} \mathbf{w} - \mathbf{P}_{S_j} \mathbf{w}^{\text{target}}\|^2, \end{aligned} \quad (\text{A24})$$

where $\bar{B}$ is the number of unique weights in the diagonal matrix $\mathbf{B}$, i.e., unique material parameters, and S_j is the subspace only containing grid points with material parameters B_j . Here, we need to assume that $\mathbf{B}$ is diagonal in S , which holds true for the acoustic wave equation or the isotropic Maxwell's equation. While this, in principle, allows for comparing two wave fields in the standard basis, we expect prohibitive sampling costs if the respective subspaces are small due to a loss of estimation globality (see Sec. VIA).

APPENDIX B: SOURCES

1. Proof of Lemma 1

(a) *Rotational covariance.* Since $\mathbf{w}^{\text{sym}}$ is rotationally covariant around $\mathbf{x}_0 = 0$, we have

$$\mathbf{R}(\mathbf{S}) \mathbf{w}^{\text{sym}}(\mathbf{x}) = \mathbf{w}^{\text{sym}}(\mathbf{S}\mathbf{x}), \quad \forall \mathbf{x}, \mathbf{S}, \quad (\text{B1})$$

where $\mathbf{S} \in \text{SO}(D)$ uniquely decomposes $\mathbf{R}(\mathbf{S}) \in \text{SO}(C)$.

(b) *Grid construction.* We discretize the space around $\mathbf{x}_0$ into a grid as follows:

(1) Radial coordinates: The radial distance r is discretized into A divisions r_a , where $a = 1, 2, \dots, A$.

(2) Angular coordinates: Each angular coordinate θ_i is discretized into $\Theta = A$ divisions, for $i = 1, 2, \dots, D - 1$.

(3) Grid points: Each grid point is specified by

$$\mathbf{x}_{a,\theta} = \mathbf{x}_0 + r_a \tilde{\mathbf{u}}_\theta, \quad (\text{B2})$$

where $\tilde{\mathbf{u}}_\theta$ is a unit vector determined by the angular indices $\theta = (\theta_1, \dots, \theta_{D-1})$.

(4) Total Number of Points: $N = A\Theta^{D-1} = A^D$ (for $D > 1$).

(c) *Efficient State Preparation Strategy*. We proceed with the following steps:

Step 1: Compute Reference Field Values. Select a reference direction, such as along the first coordinate axis, and compute $\mathbf{w}^{\text{sym}}(\mathbf{x}_{a,0})$ for $a = 1, 2, \dots, A$, where

$$\mathbf{x}_{a,0} = \mathbf{x}_0 + r_a \mathbf{e}_1, \quad (\text{B3})$$

and $\mathbf{e}_1$ is the unit vector along the first coordinate axis. This requires $O(A) = O(N^{1/D})$ classical evaluations of $\mathbf{w}^{\text{sym}}$.

Step 2: Prepare Reference Quantum State. Prepare the quantum state

$$|\phi\rangle = \frac{1}{\sqrt{\mathcal{N}'}} \sum_{c=1}^C \sum_{a=1}^A w_c^{\text{sym}}(\mathbf{x}_{a,0}) |c\rangle \otimes |a\rangle, \quad (\text{B4})$$

where $\mathcal{N}' = \sum_{c,a} |w_c^{\text{sym}}(\mathbf{x}_{a,0})|^2$. Since the number of terms is CA , this step requires $\tilde{O}(CA) = \tilde{O}(CN^{1/D})$ quantum gates [98–101].

Step 3: Create Superposition Over Angular Indices. Apply Hadamard gates to the angular index qubits to create the equal superposition:

$$|\Phi\rangle = |\phi\rangle \otimes \frac{1}{\sqrt{\Theta^{D-1}}} \sum_{\theta} |\theta\rangle. \quad (\text{B5})$$

Step 4: Apply Controlled Rotations. Our goal is to rotate the field components in $|\Phi\rangle$ to their correct orientations corresponding to each angular index θ . This is achieved by applying a sequence of controlled rotations, where the rotation angles are determined by the angular indices θ , and the rotations are performed in the planes spanned by pairs of coordinate axes. Specifically, we proceed as follows:

(1) Binary Representation of Angular Indices: Each angular coordinate θ_i is discretized into Θ divisions and represented using $k = \log_2(\Theta)$ qubits. For $\Theta = 2^k$, the total number of angular qubits is $(D-1)k$.

(2) Rotation Decomposition: To rotate the initial vector $\mathbf{w}^{\text{sym}}(\mathbf{x}_{a,0})$ to all possible directions $\tilde{\mathbf{u}}_\theta$, we decompose the rotation $\mathbf{R}_\theta \in \text{SO}(C)$ into a sequence of $C-1$ rotations. Specifically, we perform rotations in the $(i, i+1)$ planes for $i = 1, \dots, C-1$:

$$\mathbf{R}_\theta = \prod_{i=1}^{C-1} R_{i,i+1}(\theta_i), \quad (\text{B6})$$

where $R_{i,i+1}(\theta_i)$ is a rotation in the plane spanned by the i th and $(i+1)$ th coordinates, parameterized by the angle θ_i determined by θ .

(3) Sequence of Controlled Rotations: For each plane $(i, i+1)$, we apply controlled rotation gates $CR_{i,i+1}(\theta_i^{(m)})$ in the real plane, where m indexes the bits in the binary representation

of the angular coordinate θ_i . The rotation angles $\theta_i^{(m)}$ are defined as

$$\theta_i^{(m)} = \frac{\pi}{2^m}, \quad (\text{B7})$$

so that the cumulative rotation angle $\theta_i = \sum_{m=1}^k b_{i,m} \theta_i^{(m)}$, where $b_{i,m} \in \{0, 1\}$ is the m th bit of θ_i .

The controlled rotations are defined as

$$CR_{i,i+1}(\theta_i^{(m)}) = |0\rangle\langle 0|_{\theta_{i,m}} \otimes I^{\otimes C} + |1\rangle\langle 1|_{\theta_{i,m}} \otimes R_{i,i+1}(\theta_i^{(m)}), \quad (\text{B8})$$

where $\theta_{i,m}$ is the m th qubit of the angular index corresponding to the rotation in the $(i, i+1)$ plane. As the control qubits are in a state of equal superposition, all binary combinations of rotation angles are realized.

(4) Control and Target Qubits: The control qubits are the angular index qubits $|\theta\rangle$, and the target qubits are the field component qubits $|c\rangle$.

(d) *Gate Complexity*. The total number of controlled rotation gates required is $O(Ck)$, since for each of the $C-1$ planes, we apply k controlled rotations corresponding to the bits of the angular indices. Since $k = \log(\Theta) = \log(A)$, the total number of controlled rotations is $O(C \log(A)) = O(\frac{C}{D} \log(N))$. However, for fixed dimensions C and D , the gate complexity of implementing these rotations [102] is dominated by the complexity of initializing $|\phi\rangle$, which requires $\tilde{O}(CA) = \tilde{O}(CN^{1/D})$ quantum gates [98–101].

(e) *Final State Preparation*. After applying the sequence of controlled rotations, the state becomes

$$\begin{aligned} U_{\text{rot}} |\Phi\rangle &= \frac{1}{\sqrt{\mathcal{N}'\Theta^{D-1}}} \sum_{c'=1}^C \sum_{a=1}^A \sum_{\theta} \left(\prod_{i=1}^{C-1} R_{i,i+1}(\theta_i) \right)_{cc'} \\ &\quad \times w_{c'}^{\text{sym}}(\mathbf{x}_{a,0}) |c\rangle \otimes |a\rangle \otimes |\theta\rangle \\ &= \frac{1}{\sqrt{\mathcal{N}'\Theta^{D-1}}} \sum_{c=1}^C \sum_{a=1}^A \sum_{\theta} \\ &\quad \times w_c^{\text{sym}}(\mathbf{x}_{a,\theta}) |c\rangle \otimes |a\rangle \otimes |\theta\rangle, \end{aligned}$$

where we used the fact that $w_c^{\text{sym}}(\mathbf{x}_{a,\theta}) = (\mathbf{R}_\theta \mathbf{w}^{\text{sym}}(\mathbf{x}_{a,0}))_c$ due to the rotational covariance property. This is the desired state $|\psi\rangle$, which proves Lemma 1.

(f) *Practical Considerations*. Applying U_{rot} requires implementing rotations with angles that decrease exponentially with the number of qubits used to represent the angular coordinates. In practice, this poses challenges due to the finite precision of quantum gates. Specifically, the minimal rotation angle scales inversely with the state size A , resulting in a gate precision requirement that scales linearly with A . However, the precision requirement remains independent of C and D . This independence allows for the implementation of a larger total number of grid points $N = A^D$ without necessitating additional precision.

(g) *Numerical Implementation*. We provide numerical implementations for the 2D and 3D cases in Ref. [90]. Figure 2 shows the quantum circuits for the 2D and 3D cases that construct the radially symmetric vector field from a single ray.

2. Windowing

While different choices of windows are possible, in our implementation we use a symmetric double sigmoid function

$$W_j(t) = \frac{1}{1 + e^{-z \cdot t}} - \frac{1}{1 + e^{-z \cdot (t - (\tau_{j+1} - \tau_j))}}, \quad (\text{B9})$$

where z defines the steepness of the sigmoid functions. This function realizes overlapping windows that satisfy Eq. (36) with adaptable accuracy. In contrast to, e.g., box window functions ($z \rightarrow \infty$), sigmoid functions lead to smooth initial conditions. However, because the sigmoid functions do only converge to zero at the window boundary in the limit where $z \rightarrow \infty$, choosing a finite z provides a trade-off between source approximation accuracy and smoothness of the sections.

Note that if the windows are chosen to be adjacent block functions with no overlap ($z = \infty$), their appliance to a source-time function $f(t)$ does not increase the number of nonzero values, which need to be initialized. In this case, we would obtain the same initialization complexity as for a nonwindowed state. However, as we reduce the steepness of the windows, they begin to overlap. This increases the amount of initialized values and is, in the worst case, a multiplicative complexity increase with the number of windows J .

APPENDIX C: FINITE DIFFERENCE DISCRETIZATION FOR THE ACOUSTIC WAVE EQUATION

As an example, in this Appendix, we discuss the discretization of the acoustic wave equation using the finite difference (FD) method on a uniform, rectangular, and staggered grid [54]. We show how to build a pair of discrete gradient and divergence operators to ensure that $\hat{\mathbf{A}}^T = -\hat{\mathbf{A}}$ is anti-Hermitian (see Sec. II). We also discuss the implementation of Dirichlet and Neumann BCs on arbitrary boundaries of the domain by employing the constraints reduction introduced in Appendix D.

Recall the acoustic wave equation in pressure-velocity formulation introduced in Sec. II A:

$$\mathbf{B}_{\text{acoustic}} \frac{\partial \hat{\mathbf{w}}_{\text{acoustic}}}{\partial t} = \hat{\mathbf{A}}_{\text{acoustic}} \hat{\mathbf{w}}_{\text{acoustic}}$$

$$\left[\frac{1}{\rho(\mathbf{x})c^2(\mathbf{x})} \mathbf{0}_{1 \times D} \mathbf{0}_{D \times 1} \quad \rho(\mathbf{x}) \mathbb{1}_{D \times D} \right] \frac{\partial}{\partial t} \begin{bmatrix} u \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} 0 & -\nabla \cdot \\ -\nabla & \mathbf{0}_{D \times D} \end{bmatrix} \begin{bmatrix} u \\ \mathbf{v} \end{bmatrix}. \quad (\text{C1})$$

The FD method aims to construct the mapping $\nabla \rightarrow \mathbf{G} \in \mathbb{R}^{N_v \times N_u}$ and $\nabla \cdot \rightarrow \mathbf{D} \in \mathbb{R}^{N_u \times N_v}$ by defining the discrete versions of the gradient and divergence operators that will be applied to the discretized pressure fields $\mathbf{u}$ and $\mathbf{v}$, respectively. The gradient and divergence operators are constructed independently of the BCs and follow from the definition of the FD operator used to approximate derivatives in space. Without loss of generality, we use the first-order accurate central FD stencil to compute derivatives in the i th dimension:

$$\frac{\partial f}{\partial x_i}(\mathbf{x}) \approx \frac{f(\mathbf{x} + \frac{\Delta x_i}{2} \mathbf{e}_i) - f(\mathbf{x} - \frac{\Delta x_i}{2} \mathbf{e}_i)}{\Delta x_i}, \quad (\text{C2})$$

where $\mathbf{e}_i$ is the canonical vector and Δx_i is the grid step size in the i th direction. The gradient and divergence operators are

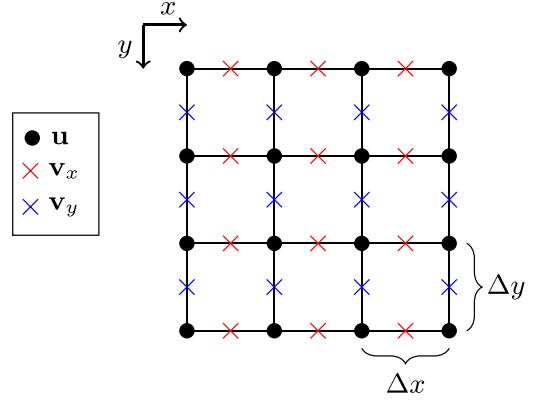


FIG. 3. Staggered grid visualization for 2D pressure-velocity formulation.

then discretized accordingly, such that

$$(\nabla u(\mathbf{x}, t))_i = \frac{\partial u}{\partial x_i}(\mathbf{x}, t)$$

$$\approx \frac{u(\mathbf{x} + \frac{\Delta x_i}{2} \mathbf{e}_i, t) - u(\mathbf{x} - \frac{\Delta x_i}{2} \mathbf{e}_i, t)}{\Delta x_i} \quad (\text{C3})$$

and

$$\nabla \cdot \mathbf{v}(\mathbf{x}, t) = \sum_{i \in D} \frac{\partial v_i}{\partial x_i}(\mathbf{x}, t)$$

$$\approx \sum_{i \in D} \frac{v_i(\mathbf{x} + \frac{\Delta x_i}{2} \mathbf{e}_i, t) - v_i(\mathbf{x} - \frac{\Delta x_i}{2} \mathbf{e}_i, t)}{\Delta x_i}. \quad (\text{C4})$$

We now need to replace the continuous fields $u(\mathbf{x}, t) : \mathbb{R}^D \times [0, T] \rightarrow \mathbb{R}$, $\mathbf{v}(\mathbf{x}, t) : \mathbb{R}^D \times [0, T] \rightarrow \mathbb{R}^D$ with their discretized counterparts $\mathbf{u}(t) : [0, T] \rightarrow \mathbb{R}^{N_u}$, $\mathbf{v}(t) : [0, T] \rightarrow \mathbb{R}^{N_v}$ by employing a *staggered* grid where the velocities are staggered in between pressure points. We introduce the set of numbers of grid points $\mathcal{N} = \{N_i \mid i \in \{1, \dots, D\}, N_i = \# \text{ of grid points in the } i\text{th direction}\}$. Since the velocity is a vector field, we need to distinguish between velocities in different dimensions: We will use $\mathbf{v}_i$ from now on to denote the velocity acting in the i th direction, such that $\mathbf{v}_i(t) : [0, T] \rightarrow \mathbb{R}^{N_{v_i}}$ where $N_{v_i} = (N_i - 1) \prod_{j \neq i} N_j$. Notice that this discretization requires the discretized velocity field in the i th direction to have one less DOF in that direction. The pressure field $\mathbf{u}$ is discretized in $N_u = \prod_i N_i$ DOFs and the full velocity field $\mathbf{v} = [\mathbf{v}_1, \dots, \mathbf{v}_D]$ in $N_v = \sum_i ((N_i - 1) \prod_{j \neq i} N_j)$ DOFs.

1. 2D Staggered grid

We now demonstrate how the staggered grid is constructed in practice for the $D = 2$ case, though the same procedure can be extended to the general D -dimensional case.

In 2D, we have three fields: $\mathbf{u}$, $\mathbf{v}_x$, and $\mathbf{v}_y$, discretized on different grid points within a rectangular domain $\Omega = [x_0, x_1] \times [y_0, y_1]$. Figure 3 provides a visual representation of the staggered grid used. Further details on its construction are described below.

We introduce the set of all grid points for the pressure field $\mathcal{X}_u$ as follows:

$$\begin{aligned}\mathcal{X}_u &= \{(x, y) \in \Omega \mid \\ x &= x_0 + (i-1)\Delta x, \quad y = y_0 + (j-1)\Delta y, \\ \forall i &\in \{1, \dots, N_x\}, \quad \forall j \in \{1, \dots, N_y\}\},\end{aligned}\quad (\text{C5})$$

where $\Delta x = (x_1 - x_0)/(N_x - 1)$, $\Delta y = (y_1 - y_0)/(N_y - 1)$, $N_x = N_1$, and $N_y = N_2$. By staggering these points, we define the set of all grid points for the velocity field in the x direction $\mathcal{X}_{v_x}$ and the y direction $\mathcal{X}_{v_y}$ as

$$\mathcal{X}_{v_x} = \{(x + \Delta x/2, y) \in \Omega \mid (x, y) \in \mathcal{X}_u\} \quad (\text{C6})$$

and

$$\mathcal{X}_{v_y} = \{(x, y + \Delta y/2) \in \Omega \mid (x, y) \in \mathcal{X}_u\}. \quad (\text{C7})$$

Notice that $|\mathcal{X}_u| = N_u = N_x N_y$, $|\mathcal{X}_{v_x}| = N_{v_x} = (N_x - 1)N_y$, and $|\mathcal{X}_{v_y}| = N_{v_y} = N_x(N_y - 1)$.

The mappings from the linear indices of the discretized fields to the grid points are given by $\Phi_u = \Phi_u(\ell) : \{1, \dots, N_u\} \rightarrow \mathcal{X}_u$, $\Phi_{v_x} = \Phi_{v_x}(k) : \{1, \dots, N_{v_x}\} \rightarrow \mathcal{X}_{v_x}$, and $\Phi_{v_y} = \Phi_{v_y}(k) : \{N_{v_x} + 1, \dots, N_{v_x} + N_{v_y}\} \rightarrow \mathcal{X}_{v_y}$. These mappings are constructed such that each index k corresponds to one and only one grid point. For example, to map the pressure points, we introduce the Cartesian indices (i, j) referring to the grid point at some position $(x_i, y_j) \in \mathcal{X}_u$, and then linearize the Cartesian index using $k = i + (j - 1)N_x$, so that $\Phi_u(\ell) = (x_i, y_j)$. A similar linearization can be performed for the velocity mappings Φ_{v_x} and Φ_{v_y} .

We now have all the necessary components to explicitly formulate the semidiscretization of pressure and velocities:

$$\begin{aligned}[\mathbf{u}]_\ell(t) &= u(\Phi_u(\ell), t), \quad \forall \ell \in \{1, \dots, N_u\}, \\ [\mathbf{v}_x]_k(t) &= v_x(\Phi_{v_x}(k), t), \quad \forall k \in \{1, \dots, N_{v_x}\}, \\ [\mathbf{v}_y]_{k-N_{v_x}}(t) &= v_y(\Phi_{v_y}(k), t), \\ &\quad \forall k \in \{N_{v_x} + 1, \dots, N_{v_x} + N_{v_y}\}.\end{aligned}\quad (\text{C8})$$

2. Discrete gradient and divergence operators, and their antitranspose relationship

We construct the discretized gradient and divergence operators in 2D based on the first-order accurate central FD scheme introduced earlier. Generalization to FD schemes with higher orders of accuracy is straightforward since the symmetry of the FD operators is retained. Therefore, the results from this section remain unchanged when using higher-order schemes.

Let $(\mathbf{G})_{k\cdot}$ denote the k th row of the gradient operator $\mathbf{G}$. When taking the dot product of this row with the discretized pressure field $\mathbf{u}$, the FD approximation of a component of the gradient ∇u is computed for the semidiscrete equation concerning the discretized velocity field component $[\mathbf{v}]_k$. If k refers to a discretized velocity component in the x direction (i.e., $k \in \{1, \dots, N_{v_x}\}$), the x component of the gradient is computed; otherwise, the y component is computed.

This can be expressed by the following FD approximation:

$$\begin{aligned}(\nabla u)_x(\Phi_{v_x}(k)) &= \frac{\partial u}{\partial x}(\Phi_{v_x}(k)) \\ &\approx \frac{u(\Phi_{v_x}(k) + \frac{\Delta x}{2}\mathbf{e}_x) - u(\Phi_{v_x}(k) - \frac{\Delta x}{2}\mathbf{e}_x)}{\Delta x} \\ &\approx \frac{u(\Phi_u(\ell_+)) - u(\Phi_u(\ell_-))}{\Delta x} \\ &\approx \frac{[\mathbf{u}]_{\ell_+} - [\mathbf{u}]_{\ell_-}}{\Delta x},\end{aligned}\quad (\text{C9})$$

for all $k \in \{1, \dots, N_{v_x}\}$. Similarly, for the y component

$$\begin{aligned}(\nabla u)_y(\Phi_{v_y}(k)) &= \frac{\partial u}{\partial y}(\Phi_{v_y}(k)) \\ &\approx \frac{u(\Phi_{v_y}(k) + \frac{\Delta y}{2}\mathbf{e}_y) - u(\Phi_{v_y}(k) - \frac{\Delta y}{2}\mathbf{e}_y)}{\Delta y} \\ &\approx \frac{u(\Phi_u(\ell_+)) - u(\Phi_u(\ell_-))}{\Delta y} \\ &\approx \frac{[\mathbf{u}]_{\ell_+} - [\mathbf{u}]_{\ell_-}}{\Delta y},\end{aligned}\quad (\text{C10})$$

for all $k \in \{N_{v_x} + 1, \dots, N_{v_x} + N_{v_y}\}$.

For each equation $k \in \{1, \dots, N_{v_x}\}$ (respectively, $k \in \{N_{v_x} + 1, \dots, N_{v_x} + N_{v_y}\}$), there will be only two nonzero coefficients in the row $(\mathbf{G})_{k\cdot}$, specifically those associated with discretized pressure components matching $\Phi_u(\ell_\pm) = \Phi_{v_x}(k) \pm (\Delta x/2)\mathbf{e}_x$ (respectively, $\Phi_u(\ell_\pm) = \Phi_{v_y}(k) \pm (\Delta y/2)\mathbf{e}_y$). Here, $\ell_\pm$ represents the index of the discretized pressure component $[\mathbf{u}]_{\ell_\pm}$. These coefficients are $\pm 1/\Delta x$ (respectively, $\pm 1/\Delta y$).

With these observations, we can explicitly write each component of the gradient operator as follows:

$$\begin{aligned}\nabla \rightarrow \mathbf{G} &= (\mathbf{G})_{k,\ell} \\ &= \begin{cases} \pm 1/\Delta x, & \text{if } k \in \{1, \dots, N_{v_x}\} \\ & \text{and } \Phi_u(\ell) = \Phi_{v_x}(k) \pm \frac{\Delta x}{2}\mathbf{e}_x, \\ \pm 1/\Delta y, & \text{if } k \in \{N_{v_x} + 1, \dots, N_{v_x} + N_{v_y}\} \\ & \text{and } \Phi_u(\ell) = \Phi_{v_y}(k) \pm \frac{\Delta y}{2}\mathbf{e}_y, \\ 0, & \text{otherwise,} \end{cases}\end{aligned}\quad (\text{C11})$$

for all $k \in \{1, \dots, N_v\}$, $\ell \in \{1, \dots, N_u\}$.

We can apply a similar procedure for the divergence operator using the FD approximation:

$$\begin{aligned}\nabla \cdot \mathbf{v}(\Phi_u(\ell)) &= \frac{\partial v_x}{\partial x}(\Phi_u(\ell)) + \frac{\partial v_y}{\partial y}(\Phi_u(\ell)) \\ &\approx \frac{v_x(\Phi_u(\ell) + \frac{\Delta x}{2}\mathbf{e}_x) - v_x(\Phi_u(\ell) - \frac{\Delta x}{2}\mathbf{e}_x)}{\Delta x} \\ &\quad + \frac{v_y(\Phi_u(\ell) + \frac{\Delta y}{2}\mathbf{e}_y) - v_y(\Phi_u(\ell) - \frac{\Delta y}{2}\mathbf{e}_y)}{\Delta y}\end{aligned}$$

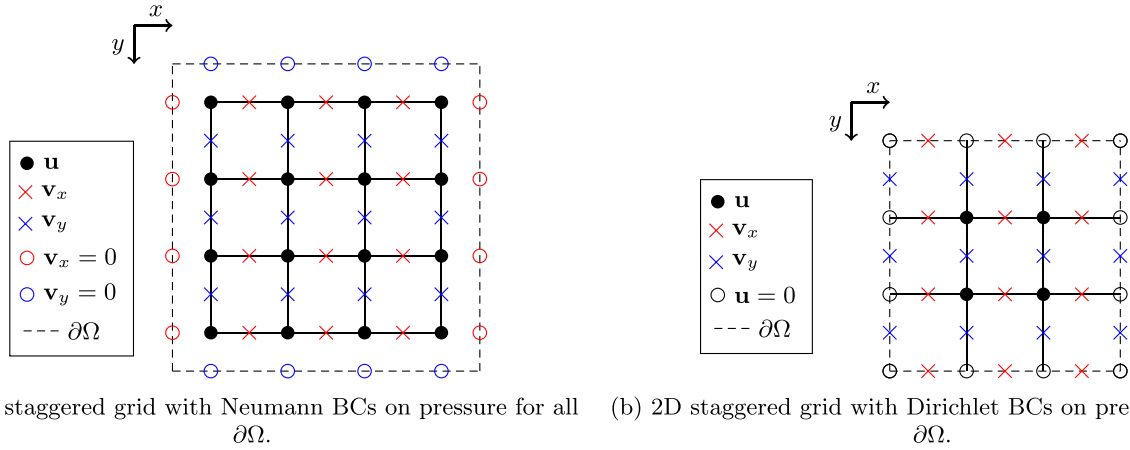


FIG. 4. Examples of different boundary condition implementations.

$$\begin{aligned}
&\approx \frac{v_x(\Phi_{v_x}(k_{x+})) - v_x(\Phi_{v_x}(k_{x-}))}{\Delta x} \\
&+ \frac{v_y(\Phi_{v_y}(k_{y+})) - v_y(\Phi_{v_y}(k_{y-}))}{\Delta y} \\
&\approx \frac{[\mathbf{v}_x]_{k_{x+}} - [\mathbf{v}_x]_{k_{x-}}}{\Delta x} \\
&+ \frac{[\mathbf{v}_y]_{k_{y+}} - [\mathbf{v}_y]_{k_{y-}}}{\Delta y}, \tag{C12}
\end{aligned}$$

resulting in

$$\begin{aligned}
&\nabla \cdot \rightarrow \mathbf{D} = (\mathbf{D})_{\ell,k} \\
&= \begin{cases} \pm 1/\Delta x, & \text{if } k \in \{1, \dots, N_{v_x}\} \\ & \text{and } \Phi_{v_x}(k) = \Phi_u(\ell) \pm \frac{\Delta x}{2} \mathbf{e}_x, \\ \pm 1/\Delta y, & \text{if } k \in \{N_{v_x} + 1, \dots, N_{v_x} + N_{v_y}\} \\ & \text{and } \Phi_{v_y}(k) = \Phi_u(\ell) \pm \frac{\Delta y}{2} \mathbf{e}_y, \\ 0, & \text{otherwise.} \end{cases} \tag{C13}
\end{aligned}$$

The antitranspose property $\mathbf{G} = -\mathbf{D}^T$ can be verified by showing that $(\mathbf{G})_{k,\ell} = -(\mathbf{D})_{\ell,k}$ for all ℓ, k . This is easily checked by observing that the only difference in the definition of the operators $\mathbf{G}$ and $\mathbf{D}$ is the position of the mappings Φ_u and Φ_{v_x} (respectively, Φ_u and Φ_{v_y}) in

the conditions $\Phi_u(\ell) = \Phi_{v_x}(k) \pm (\Delta x/2)\mathbf{e}_x$ and $\Phi_{v_x}(k) = \Phi_u(\ell) \pm (\Delta x/2)\mathbf{e}_x$ [respectively, the conditions $\Phi_u(\ell) = \Phi_{v_y}(k) \pm (\Delta y/2)\mathbf{e}_y$ and $\Phi_{v_y}(k) = \Phi_u(\ell) \pm (\Delta y/2)\mathbf{e}_y$], which is the cause of sign flip of the components. This shows that the FD discretization using a uniform, rectangular, staggered grid produces a pair of gradient and divergence operators leading to an anti-Hermitian matrix $\mathbf{A} = \begin{bmatrix} \mathbf{0}_{N_u \times N_u} & -\mathbf{D} \\ -\mathbf{G} & \mathbf{0}_{D \times D} \end{bmatrix}$.

3. Implementation of boundary conditions

The staggered grid described in the previous section naturally implements Neumann BCs, as the velocities in the direction perpendicular to the domain's boundaries are assumed to be vanishing, i.e., $\mathbf{v}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0$ for all $\mathbf{x} \in \partial\Omega$, where $\mathbf{n}(\mathbf{x})$ is the normal vector at position $\mathbf{x}$ on the boundary $\partial\Omega$. A visual representation is shown in Fig. 4(a), where the actual boundaries of the domain are depicted with a dashed line. To implement Dirichlet BCs, i.e., $\mathbf{u}(\mathbf{x}) = 0$ for all $\mathbf{x} \in \partial\Omega$, constraints on pressure points with indices in the set $\{\ell \mid \Phi_u(\ell) \in \partial\Omega\}$ must be added. Figure 4(b) provides a visual representation of these constraints. Using the method presented in Appendix D, we can employ Dirichlet or Neumann BCs along arbitrary boundaries that align with the grid. An example for a rectangular

grid with changing boundary conditions is displayed in Fig. 4(c).

Since these added constraints result in a system where $\mathbf{R}_f = 0$ (see Appendix D), i.e., the unconstrained DOFs do not appear in the constraint matrix $\mathbf{R}$, the modified matrices will be $\underline{\mathbf{B}} = \mathbf{B}_{ff}$ and $\underline{\mathbf{A}} = \mathbf{A}_{ff}$, which are the original with some rows and columns removed corresponding to the newly constrained DOFs.

Because the matrices $\mathbf{B}$ and $\mathbf{A}$ were Hermitian and anti-Hermitian by construction, respectively, the modified matrices $\underline{\mathbf{B}}$ and $\underline{\mathbf{A}}$ will remain Hermitian and anti-Hermitian, since deleting one row and column corresponding to the same index of a Hermitian (or anti-Hermitian) matrix results in a matrix that is still Hermitian (or anti-Hermitian).

APPENDIX D: GENERALIZING BOUNDARY CONDITIONS TO LINEAR CONSTRAINTS

In Appendix C3, we showed that in the acoustic case and for rectangular domains Neumann or Dirichlet BCs emerge naturally. In this Appendix, we introduce a general method to deal with BCs. The method operates directly on the discretized but general wave equation

$$\mathbf{B} \frac{d\mathbf{w}(t)}{dt} = \mathbf{A}\mathbf{w}(t), \quad (\text{D1})$$

where we aim to impose BCs as constraints. These constraints modify the wave equation and can introduce source terms. We assume that these constraints can be expressed in the following form:

$$\mathbf{R}\mathbf{w} = [\mathbf{R}_f, \mathbf{R}_c] \begin{bmatrix} \mathbf{w}_f \\ \mathbf{w}_c \end{bmatrix} = \mathbf{b}(t), \quad (\text{D2})$$

where $\mathbf{R} \in \mathbb{R}^{N_c \times N}$ is the constraint matrix, N_c is the number of constraints, $\mathbf{w}_f \in \mathbb{R}^{N-N_c}$ represents the free (unconstrained) DOFs, and $\mathbf{w}_c \in \mathbb{R}^{N_c}$ represents the constrained DOFs, which will be eliminated from the equations of motion. The vector $\mathbf{b}(t)$ is nonzero if the constraints are nonhomogeneous. For example, in a 2D acoustic wave problem with FD discretization, homogeneous Dirichlet (Neumann) BCs along any boundary orthogonal to the x or y velocity components can be enforced by setting $\mathbf{b}_i = 0$, $\mathbf{R}_f = \mathbf{0}$, and $\mathbf{R}_c = \mathbf{1}$ for all pressure (velocity) values on the boundary.

To incorporate the BCs (or constraints) into the wave equation, we follow the approach in Ref. [57]. We solve for the constrained DOFs

$$\mathbf{w}_c = -\mathbf{R}_c^{-1} \mathbf{R}_f \mathbf{w}_f + \mathbf{R}_c^{-1} \mathbf{b}(t). \quad (\text{D3})$$

Next, we rearrange the equations of motion to separate the free and constrained components:

$$\begin{bmatrix} \mathbf{B}_{ff} & \mathbf{B}_{fc} \\ \mathbf{B}_{cf} & \mathbf{B}_{cc} \end{bmatrix} \frac{d}{dt} \begin{bmatrix} \mathbf{w}_f \\ \mathbf{w}_c \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{ff} & \mathbf{A}_{fc} \\ \mathbf{A}_{cf} & \mathbf{A}_{cc} \end{bmatrix} \begin{bmatrix} \mathbf{w}_f \\ \mathbf{w}_c \end{bmatrix}. \quad (\text{D4})$$

Rearranging the equations in this way preserves the Hermitian or anti-Hermitian nature of the matrices. Substituting Eq. (D3) into the above equation and solving for the free DOFs yields

$$\underline{\mathbf{B}} \frac{d\mathbf{w}_f(t)}{dt} = \underline{\mathbf{A}}\mathbf{w}_f(t) + \underline{\mathbf{s}}_c(t), \quad (\text{D5})$$

where

$$\underline{\mathbf{B}} = \mathbf{B}_{ff} - \mathbf{B}_{fc} \mathbf{R}_c^{-1} \mathbf{R}_f \quad (\text{D6})$$

and

$$\underline{\mathbf{A}} = \mathbf{A}_{ff} - \mathbf{A}_{fc} \mathbf{R}_c^{-1} \mathbf{R}_f. \quad (\text{D7})$$

For the constraints to be compatible with this approach, $\underline{\mathbf{B}}$ and $\underline{\mathbf{A}}$ must be Hermitian and anti-Hermitian, respectively. This condition is automatically satisfied when $\mathbf{R}_f = \mathbf{0}$. In other cases, these conditions can be used to assess whether the constraints are implementable using an HS scheme, which relies on the Hermitian or anti-Hermitian properties of the matrices. The source term is given by

$$\underline{\mathbf{s}}_c(t) = \mathbf{A}_{fc} \mathbf{R}_c^{-1} \mathbf{b}(t) - \mathbf{B}_{fc} \mathbf{R}_c^{-1} \frac{d\mathbf{b}(t)}{dt}. \quad (\text{D8})$$

In general, this source cannot be implemented within our framework as the resulting wave field that needs to be initialized is neither radially symmetric nor populates a volume that is independent of N . However, if $\mathbf{b}(t)$ is pulselike and a point source in space, then the logic of Sec. VA applies, giving rise to a quantum initialization that is independent of N . Hence, certain boundary or displacement control problems can be implemented within the presented framework.

In summary, this scheme offers a practical approach to implementing BCs: First, discretize the equations, ensuring that the operators maintain the necessary Hermitian or anti-Hermitian properties, and then introduce the BCs along the chosen boundaries as described.

Finally, absorbing boundaries or perfectly matched layers have played a crucial role in computational wave physics [1,103,104]. Due to their fundamentally nonenergy conserving nature, it is not straightforward to implement such BCs on a QC within the HS framework. However, they can approximately be implemented using random boundaries that diffuse the wave field, thereby minimizing the energy that is backscattered into the volume of interest [105,106].

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- [1] A. Fichtner, *Full Seismic Waveform Modelling and Inversion, Advances in Geophysical and Environmental Mechanics and Mathematics* (Springer, Berlin, Germany, 2011)
 - [2] S. Cesca and F. Grigoli, Full Waveform Seismological Advances for Microseismic Monitoring, in *Advances in Geophysics*, edited by R. Dmowska (Elsevier, Amsterdam, Netherlands, 2015), Vol. 56, Chap. 2, pp. 169–228.

- [3] H. Igel, *Computational Seismology: A Practical Introduction* (Oxford University Press, Oxford, UK, 2017).
- [4] S. J. Arrowsmith, D. T. Trugman, J. MacCarthy, K. J. Bergen, D. Lumley, and M. B. Magnani, Big data seismology, *Rev. Geophys.* **60**, e2021RG000769 (2022).
- [5] R. G. Pratt, L. Huang, N. Duric, and P. Littrup, Sound-speed and attenuation imaging of breast tissue using waveform

- tomography of transmission ultrasound data, in *Medical Imaging 2007: Physics of Medical Imaging*, edited by J. Hsieh and M. J. Flynn (SPIE, Bellingham, Washington, USA, 2007), Vol. 6510, pp. 1523–1534.
- [6] H. Gemmeke and N. V. Ruiter, 3D ultrasound computer tomography for medical imaging, *Nucl. Instrum. Methods Phys. Res. Sect. A* **580**, 1057 (2007).
- [7] *Ultrasound Imaging: Advances and Applications*, edited by J. M. Sanches, A. F. Laine, and J. S. Suri (Springer, Berlin, Heidelberg, Germany, 2012).
- [8] S. Ould Naffa, M. Goueygou, B. Piwakowski, and F. Buyle-Bodin, Detection of chemical damage in concrete using ultrasound, *Ultrasonics* **40**, 247 (2002).
- [9] K. Kim and W. R. Wagner, Non-invasive and non-destructive characterization of tissue engineered constructs using ultrasound imaging technologies: A review, *Ann. Biomed. Eng.* **44**, 621 (2016).
- [10] A. Lopez, R. Bacelar, I. Pires, T. G. Santos, J. P. Sousa, and L. Quintino, Non-destructive testing application of radiography and ultrasound for wire and arc additive manufacturing, *Addit. Manuf.* **21**, 298 (2018).
- [11] M. P. Bendsoe and O. Sigmund, *Topology Optimization: Theory, Methods, and Applications* (Springer Science & Business Media, Berlin, Germany, 2013).
- [12] R. E. Christiansen and O. Sigmund, Inverse design in photonics by topology optimization: tutorial, *J. Opt. Soc. Am. B* **38**, 496 (2021).
- [13] A. K. Sharma, M. Kosta, G. Shmuel, and O. Amir, Gradient-based topology optimization of soft dielectrics as tunable phononic crystals, *Compos. Struct.* **280**, 114846 (2022).
- [14] G. Bordiga, E. Medina, S. Jafarzadeh, C. Bösch, R. P. Adams, V. Tournat, and K. Bertoldi, Automated discovery of reprogrammable nonlinear dynamic metamaterials, *Nat. Mater.* **23**, 1486 (2024).
- [15] Ö. Yilmaz, *Seismic Data Analysis* (Society of Exploration Geophysicists, Houston, Texas, USA, 2001).
- [16] A. Fichtner and J. Trampert, Resolution analysis in full waveform inversion, *Geophys. J. Int.* **187**, 1604 (2011).
- [17] N. Rawlinson, A. Fichtner, M. Sambridge, and M. K. Young, Seismic tomography and the assessment of uncertainty, in *Advances in Geophysics*, edited by R. Dmowska (Elsevier, Amsterdam, Netherlands, 2014), Vol. 55, Chap. 1, pp. 1–76.
- [18] M. Betancourt, A conceptual introduction to Hamiltonian Monte Carlo, *arXiv:1701.02434*.
- [19] M. K. Sen and R. Biswas, Transdimensional seismic inversion using the reversible jump Hamiltonian Monte Carlo algorithm, *Geophysics* **82**, R119 (2017).
- [20] A. Fichtner, A. Zunino, and L. Gebraad, Hamiltonian Monte Carlo solution of tomographic inverse problems, *Geophys. J. Int.* **216**, 1344 (2019).
- [21] I. E. Ulrich, C. Boehm, A. Zunino, and A. Fichtner, Analyzing resolution and model uncertainties for ultrasound computed tomography using Hessian information, in *Medical Imaging 2022: Ultrasonic Imaging and Tomography*, edited by N. Botenous and N. V. Ruiter (SPIE, Bellingham, Washington, 2022), Vol. 12038, pp. 48–60.
- [22] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, UK, 2010), 10th ed.
- [23] A. Montanaro, Quantum algorithms: An overview, *npj Quantum Inf.* **2**, 15023 (2016).
- [24] M. Cerezo, A. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio, and P. J. Coles, Variational quantum algorithms, *Nat. Rev. Phys.* **3**, 625 (2021).
- [25] J. M. Martyn, Z. M. Rossi, A. K. Tan, and I. L. Chuang, Grand unification of quantum algorithms, *PRX Quantum* **2**, 040203 (2021).
- [26] A. M. Childs and N. Wiebe, Hamiltonian simulation using linear combinations of unitary operations, *arXiv:1202.5822*.
- [27] G. H. Low and I. L. Chuang, Optimal Hamiltonian simulation by quantum signal processing, *Phys. Rev. Lett.* **118**, 010501 (2017).
- [28] G. H. Low and I. L. Chuang, Hamiltonian simulation by qubitization, *Quantum* **3**, 163 (2019).
- [29] G. H. Low, Y. Su, Y. Tong, and M. C. Tran, Complexity of implementing trotter steps, *PRX Quantum* **4**, 020323 (2023).
- [30] P. C. S. Costa, S. Jordan, and A. Ostrander, Quantum algorithm for simulating the wave equation, *Phys. Rev. A* **99**, 012323 (2019).
- [31] A. Suau, G. Staffelbach, and H. Calandra, Practical quantum computing: Solving the wave equation using a quantum approach, *ACM Trans. Quantum Comput.* **2**, 1 (2021).
- [32] E. Koukoutsis, K. Hizanidis, A. K. Ram, and G. Vahala, Dyson maps and unitary evolution for Maxwell equations in tensor dielectric media, *Phys. Rev. A* **107**, 042215 (2023).
- [33] Y. Sato, R. Kondo, I. Hamamura, T. Onodera, and N. Yamamoto, Hamiltonian simulation for hyperbolic partial differential equations by scalable quantum circuits, *Phys. Rev. Res.* **6**, 033246 (2024).
- [34] Y. Sato, H. Tezuka, R. Kondo, and N. Yamamoto, Quantum algorithm for partial differential equations of nonconservative systems with spatially varying parameters, *Phys. Rev. Appl.* **23**, 014063 (2025).
- [35] M. Schade, C. Bösch, V. Hapla, and A. Fichtner, A quantum computing concept for 1-D elastic wave simulation with exponential speedup, *Geophys. J. Int.* **238**, 321 (2024).
- [36] R. Babbush, D. W. Berry, R. Kothari, R. D. Somma, and N. Wiebe, Exponential quantum speedup in simulating coupled classical oscillators, *Phys. Rev. X* **13**, 041041 (2023).
- [37] Y. Ito, Y. Tanaka, and K. Fujii, How to map linear differential equations to Schrödinger equations via Carleman and Koopman-von Neumann embeddings for quantum algorithms, *arXiv:2311.15628*.
- [38] S. Danz, M. Berta, S. Schröder, P. Kienast, F. K. Wilhelm, and A. Ciani, Calculating response functions of coupled oscillators using quantum phase estimation, *Phys. Rev. Res.* **7**, 023264 (2025).
- [39] S. Jin, N. Liu, and C. Ma, Quantum simulation of Maxwell's equations via Schrödingerisation, *ESAIM: Math. Modell. Numer. Anal.* **58**, 1853 (2024).
- [40] S. Jin, N. Liu, and Y. Yu, Quantum simulation of partial differential equations: Applications and detailed analysis, *Phys. Rev. A* **108**, 032603 (2023).
- [41] C. Ma, S. Jin, N. Liu, K. Wang, and L. Zhang, Schrödingerization based quantum circuits for maxwell's equation with time-dependent source terms, *arXiv:2411.10999*.

- [42] S. G. Johnson, Notes on the algebraic structure of wave equations (2007), <https://math.mit.edu/~stevenj/18.369/wave-equations.pdf>.
- [43] A. Mostafazadeh, Pseudo-Hermitian representation of quantum mechanics, *Int. J. Geom. Methods Mod. Phys.* **07**, 1191 (2010).
- [44] M. Kaltenbacher, *Fundamental equations of acoustics*, in *Computational Acoustics* (Springer International Publishing, Springer Berlin, Germany, 2018), p. 12.
- [45] D. J. Griffiths, *Introduction to Electrodynamics* (Cambridge University Press, Cambridge, UK, 2023).
- [46] S. G. Johnson and J. D. Joannopoulos, *Photonic Crystals: The Road from Theory to Practice* (Springer Science & Business Media, Berlin, Germany, 2001).
- [47] J. Jackson, *Classical Electrodynamics* (John Wiley & Sons, Hoboken, New Jersey, USA, 2021).
- [48] H.-L. Liu, Y.-S. Wu, L.-C. Wan, S.-J. Pan, S.-J. Qin, F. Gao, and Q.-Y. Wen, Variational quantum algorithm for the Poisson equation, *Phys. Rev. A* **104**, 022418 (2021).
- [49] Y. Sato, R. Kondo, S. Koide, H. Takamatsu, and N. Imoto, Variational quantum algorithm based on the minimum potential energy for solving the Poisson equation, *Phys. Rev. A* **104**, 052409 (2021).
- [50] W. Voigt, *Lehrbuch der Kristallphysik* (Vieweg und Teubner Verlag, Wiesbaden, Germany, 1966).
- [51] C. Scheibner, A. Souslov, D. Banerjee, P. Surówka, W. T. M. Irvine, and V. Vitelli, Odd elasticity, *Nat. Phys.* **16**, 475 (2020).
- [52] K. Aki and P. G. Richards, *Quantitative Seismology* (University Science Books, Melville, New York, USA, 2002), 2nd ed.
- [53] L. Landau, L. Pitaevskii, A. Kosevich, and E. Lifshitz, *Theory of Elasticity* (Butterworth-Heinemann, Oxford, UK, 2012), Vol. 7, Bd. 7.
- [54] J. Virieux, SH-wave propagation in heterogeneous media; velocity-stress finite-difference method, *Geophysics* **49**, 1933 (1984).
- [55] K. Yee, Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media, *IEEE Trans. Antennas Propag.* **14**, 302 (1966).
- [56] A. Taflov, S. C. Hagness, and M. Piket-May, Computational electromagnetics: The finite-difference time-domain method, in *The Electrical Engineering Handbook*, edited by W.-K. Chen (Academic Press, Burlington, 2005), pp. 629–670.
- [57] J. Hoepffner, Implementation of boundary conditions (2007), <https://www.google.com/url?sa=t&source=web&rct=j&opi=89978449&url=http://www.lmm.jussieu.fr/~hoepffner/boundarycondition.pdf&ved=2ahUKEwiT6LbkoZmPAxUx0QIHUoEBXsQFnoECBUQAQ&usg=AOvVaw0alHuBliTPd4iOdkdTkZtr>.
- [58] L. Banjai and S. Sauter, Rapid solution of the wave equation in unbounded domains, *SIAM J. Numer. Anal.* **47**, 227 (2009).
- [59] Z.-G. Qian and W. C. Chew, Fast full-wave surface integral equation solver for multiscale structure modeling, *IEEE Trans. Antennas Propag.* **57**, 3594 (2009).
- [60] J.-G. Wei, Z. Peng, and J.-F. Lee, A fast direct matrix solver for surface integral equation methods for electromagnetic wave scattering from non-penetrable targets, *Radio Sci.* **47**, 2012RS004988 (2012).
- [61] S. Omar and D. Jiao, A linear complexity direct volume integral equation solver for full-wave 3-D circuit extraction in inhomogeneous materials, *IEEE Trans. Microwave Theory Tech.* **63**, 897 (2015).
- [62] F. Smith, S. Tsynkov, and E. Turkel, Compact high order accurate schemes for the three dimensional wave equation, *J. Sci. Comput.* **81**, 1181 (2019).
- [63] A. V. Oppenheim, A. S. Willsky, and S. H. Nawab, *Signals & Systems* (Pearson Educación, London, UK, 1997).
- [64] C. Johnson, Finite element methods for linear hyperbolic problems, *Comput. Methods Appl. Mech. Eng.* **45**, 285 (1984).
- [65] R. J. LeVeque, *Finite Volume Methods for Hyperbolic Problems* (Cambridge University Press, Cambridge, UK, 2002).
- [66] J. C. Strikwerda, *Finite Difference Schemes and Partial Differential Equations* (SIAM, Philadelphia, Pennsylvania, United States, 2004).
- [67] J. Crank and P. Nicolson, A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type, *Math. Proc. Cambridge Philos. Soc.* **43**, 50 (1947).
- [68] D. Camps, L. Lin, R. Van Beeumen, and C. Yang, Explicit quantum circuits for block encodings of certain sparse matrices, *SIAM J. Matrix Anal. Appl.* **45**, 801 (2024).
- [69] S. Ty, R. Vilmart, A. TahmasebiMoradi, and C. Mang, Double-logarithmic depth block-encodings of simple finite difference method's matrices, [arXiv:2410.05241](https://arxiv.org/abs/2410.05241).
- [70] C. Sünderhauf, E. Campbell, and J. Camps, Block-encoding structured matrices for data input in quantum computing, *Quantum* **8**, 1226 (2024).
- [71] N. Guseynov, X. Huang, and N. Liu, Gate construction of block-encoding for Hamiltonians needed for simulating partial differential equations, *Phys. Rev. Res.* **7**, 033100 (2025).
- [72] J. Welch, D. Greenbaum, S. Mostame, and A. Aspuru-Guzik, Efficient quantum circuits for diagonal unitaries without ancillas, *New J. Phys.* **16**, 033040 (2014).
- [73] M. R. Garey, D. S. Johnson, and L. Stockmeyer, Some simplified np-complete problems, in *Proceedings of the Sixth Annual ACM Symposium on Theory of Computing, STOC '74* (Association for Computing Machinery, New York, USA, 1974), pp. 47–63.
- [74] L. Grover and T. Rudolph, Creating superpositions that correspond to efficiently integrable probability distributions, [arXiv:quant-ph/0208112](https://arxiv.org/abs/quant-ph/0208112).
- [75] A. W. Harrow and A. Y. Wei, Adaptive quantum simulated annealing for bayesian inference and estimating partition functions, in *Proceedings of the 2020 ACM-SIAM Symposium on Discrete Algorithms (SODA)* (SIAM, Philadelphia, Pennsylvania, United States, 2019), pp. 193–212.
- [76] P. Rall and B. Fuller, Amplitude estimation from quantum signal processing, *Quantum* **7**, 937 (2023).
- [77] H. Krovi, Quantum algorithms to simulate quadratic classical Hamiltonians and optimal control, [arXiv:2404.07303](https://arxiv.org/abs/2404.07303).
- [78] E. Koukoutsis, K. Hizanidis, A. K. Ram, and G. Vahala, Quantum simulation of dissipation for Maxwell equations in dispersive media, *Future Gener. Comput. Syst.* **159**, 221 (2024).
- [79] Z. Hu, R. Xia, and S. Kais, A quantum algorithm for evolving open quantum dynamics on quantum computing devices, *Sci. Rep.* **10**, 3301 (2020).

- [80] D. An, J.-P. Liu, and L. Lin, Linear combination of Hamiltonian simulation for nonunitary dynamics with optimal state preparation cost, *Phys. Rev. Lett.* **131**, 150603 (2023).
- [81] D. An, A. M. Childs, and L. Lin, Quantum algorithm for linear non-unitary dynamics with near-optimal dependence on all parameters, [arXiv:2312.03916](https://arxiv.org/abs/2312.03916).
- [82] H. Nassar, H. Chen, A. N. Norris, and G. L. Huang, Quantization of band tilting in modulated phononic crystals, *Phys. Rev. B* **97**, 014305 (2018).
- [83] H. Chen, L. Yao, H. Nassar, and G. Huang, Mechanical quantum Hall effect in time-modulated elastic materials, *Phys. Rev. Appl.* **11**, 044029 (2019).
- [84] E. Galiffi, R. Tirole, S. Yin, H. Li, S. Vezzoli, P. A. Huidobro, M. G. Silveirinha, R. Sapienza, A. Alù, and J. B. Pendry, Photonics of time-varying media, *Adv. Photonics* **4**, 014002 (2022).
- [85] C. Bösch, A. Fichtner, and M. Serra-Garcia, Differences between quantum and classical adiabatic evolution, *Phys. Rev. B* **110**, 064307 (2024).
- [86] L. Clinton, J. Bausch, and T. Cubitt, Hamiltonian simulation algorithms for near-term quantum hardware, *Nat. Commun.* **12**, 4989 (2021).
- [87] Y. Kikuchi, C. Mc Keever, L. Coopmans, M. Lubasch, and M. Benedetti, Realization of quantum signal processing on a noisy quantum computer, *npj Quantum Inf.* **9**, 93 (2023).
- [88] L. Wright, C. Mc Keever, J. T. First, R. Johnston, J. Tillay, S. Chaney, M. Rosenkranz, and M. Lubasch, Noisy intermediate-scale quantum simulation of the one-dimensional wave equation, *Phys. Rev. Res.* **6**, 043169 (2024).
- [89] R. Acharya *et al.* (Google Quantum AI and Collaborators), Quantum error correction below the surface code threshold, *Nature (London)* **638**, 920 (2025).
- [90] C. Bösch, M. Schade, G. Aloisi, S. D. Keating, and A. Fichtner, Code: Quantum wave simulation with sources and loss functions (2025), <https://github.com/malteschade/>.
- [91] R. Iten, R. Colbeck, I. Kukuljan, J. Home, and M. Christandl, Quantum circuits for isometries, *Phys. Rev. A* **93**, 032318 (2016).
- [92] Y. He, M.-X. Luo, E. Zhang, H.-K. Wang, and X.-F. Wang, Decompositions of n -qubit Toffoli gates with linear circuit complexity, *Int. J. Theor. Phys.* **56**, 2350 (2017).
- [93] B. Zindorf and S. Bose, Efficient implementation of multi-controlled quantum gates, [arXiv:2404.02279](https://arxiv.org/abs/2404.02279).
- [94] E. A. Martinez, T. Monz, D. Nigg, P. Schindler, and R. Blatt, Compiling quantum algorithms for architectures with multi-qubit gates, *New J. Phys.* **18**, 063029 (2016).
- [95] N. Goel and J. K. Freericks, Native multiqubit Toffoli gates on ion trap quantum computers, *Quantum Sci. Technol.* **6**, 044010 (2021).
- [96] Y. Kim, A. Morvan, L. B. Nguyen, R. K. Naik, C. Jünger, L. Chen, J. M. Kreikebaum, D. I. Santiago, and I. Siddiqi, High-fidelity three-qubit iToffoli gate for fixed-frequency superconducting qubits, *Nat. Phys.* **18**, 783 (2022).
- [97] E. Knill, G. Ortiz, and R. D. Somma, Optimal quantum measurements of expectation values of observables, *Phys. Rev. A* **75**, 012328 (2007).
- [98] N. Gleinig and T. Hoefer, An efficient algorithm for sparse quantum state preparation, in *2021 58th ACM/IEEE Design Automation Conference (DAC)* (IEEE, San Francisco, CA, USA, 2021), pp. 433–438.
- [99] E. Malvetti, R. Iten, and R. Colbeck, Quantum circuits for sparse isometries, *Quantum* **5**, 412 (2021).
- [100] T. M. L. de Veras, L. D. da Silva, and A. J. da Silva, Double sparse quantum state preparation, *Quantum Inf. Proc.* **21**, 204 (2022).
- [101] X.-M. Zhang, T. Li, and X. Yuan, Quantum state preparation with optimal circuit depth: Implementations and applications, *Phys. Rev. Lett.* **129**, 230504 (2022).
- [102] R. Vale, T. M. D. Azevedo, I. C. S. Araújo, I. F. Araújo, and A. J. da Silva, Circuit decomposition of multicontrolled special unitary single-qubit gates, *IEEE Trans. Comput.-Aided Des. Integr. Circuits Syst.* **43**, 802 (2024).
- [103] R. L. Higdon, Absorbing boundary conditions for acoustic and elastic waves in stratified media, *J. Comput. Phys.* **101**, 386 (1992).
- [104] J.-P. Berenger, A perfectly matched layer for the absorption of electromagnetic waves, *J. Comput. Phys.* **114**, 185 (SEG, Houston, Texas, USA, 1994).
- [105] R. G. Clapp, Reverse time migration with random boundaries, in *SEG Technical Program Expanded Abstracts 2009* (Society of Exploration Geophysicists, 2009), pp. 2809–2813.
- [106] X. Shen and R. G. Clapp, Random boundary condition for memory-efficient waveform inversion gradient computation, *Geophysics* **80**, R351 (2015).