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## Quantum Simulation via Filtered Hamiltonian Engineering: Application to Perfect Quantum Transport in Spin Networks

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We propose a method for Hamiltonian engineering that requires no local control but only relies on collective qubit rotations and field gradients. The technique achieves a spatial modulation of the coupling strengths via a dynamical construction of a weighting function combined with a Bragg grating. As an example, we demonstrate how to generate the ideal Hamiltonian for perfect quantum information transport between two separated nodes of a large spin network. We engineer a spin chain with optimal couplings starting from a large spin network, such as one naturally occurring in crystals, while decoupling all unwanted interactions. For realistic experimental parameters, our method can be used to drive almost perfect quantum information transport at room temperature. The Hamiltonian engineering method can be made more robust under decoherence and coupling disorder by a novel apodization scheme. Thus, the method is quite general and can be used to engineer the Hamiltonian of many complex spin lattices with different topologies and interactions.

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Controlling the evolution of complex quantum systems has emerged as an important area of research for its promising applications. The control task can often be reduced to Hamiltonian engineering [1] (also extended to reservoir engineering [2–4]), which has enabled a variety of tasks, including quantum computation [5], improved quantum metrology [6], and dynamical decoupling [7–9]. The most important application is quantum simulation [10,11], with the ultimate goal to achieve a programmable universal quantum simulator that is able to mimic the dynamics of any system. One possible strategy is to use a quantum computer and decompose the desired evolution into unitary gates [12,13]. Alternatively, one can use Hamiltonian engineering by a Suzuki-Trotter factorization of the desired interaction into experimentally achievable Hamiltonians [14,15]. However, experimental implementations of these simulation methods often require local quantum control, which is difficult to achieve in large systems.

Here, we present a scheme for Hamiltonian engineering that employs only collective rotations of the qubits and field gradients—technology that is readily available, e.g., in magnetic resonance, ion traps [13], and optical lattices [16]. We consider a qubit network (Fig. 1) with an internal Hamiltonian  $\mathcal{H}_{\text{int}}$ , for example, due to dipolar couplings naturally occurring among spins in a crystal lattice. The target Hamiltonian  $\mathcal{H}_{\text{tar}}$  is engineered from  $\mathcal{H}_{\text{int}}$  by first “removing” unwanted couplings and then “modulating” the remaining coupling strengths. The first step is equivalent to creating a time-domain Bragg grating, a sharp filter that retains only specific couplings [17]. Then, a weighting function allows fine-tuning of their strengths, without the need for local control.

Hamiltonian engineering has a long history in NMR, as described by coherent averaging [18,19], and field gradients have been proposed to achieve NMR “diffraction” in solid [20,21]. While pulse sequences exist for selective excitation [22] and have been recently extended to achieve dynamical decoupling [8] and to turn on couplings one at a time [23,24], our method is more flexible and general than previous techniques. Since it achieves simultaneous tunability of the filtered coupling strengths by exploiting magnetic-field gradients and a photonics-inspired approach for robust filter construction [17], our method offers an intuitive and quantitative approach to Hamiltonian engineering in many physical settings.

As an example, we show how to apply this filtered engineering method to generate an optimal Hamiltonian for quantum information transfer (QIT). Linear arrays of spins have been proposed as quantum wires to link

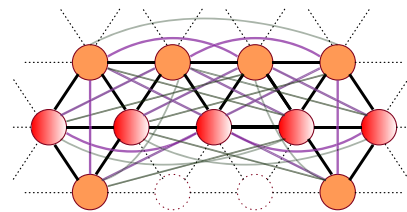


FIG. 1 (color online). A complex spin network in a trigonal planar lattice. Only spins considered in simulations are depicted with edges denoting couplings. Hamiltonian engineering preserves only NN couplings inside a chain (red circles) and eliminates off-chain couplings to the surrounding network (orange circles), thanks to a linear magnetic-field gradient along the chain.

separated nodes of a spin network [25]; engineering the coupling between the spins can achieve perfect QIT [26]. Finally, we will analyze experimental requirements to implement the method in existing physical architectures.

*Hamiltonian engineering.*—The goals of filtered Hamiltonian engineering can be summarized as (i) cancellation of unwanted couplings—often next-nearest-neighbor interactions—and (ii) engineering of the remaining couplings to match the desired coupling strengths. We achieve these goals by dynamically generating tunable and independent grating ( $\mathcal{G}_{ij}$ ) and weighting ( $F_{ij}$ ) functions via collective rotations under a gradient. The first step is to create the Hamiltonian operator one wishes to simulate using sequences of collective pulses. Although the initial Hamiltonian  $\mathcal{H}_{\text{int}}$  restricts which operators can be obtained [27], various control sequences have been proposed to realize a broad set of Hamiltonians [28,29]. These multiple-pulse sequences cannot, however, modulate specific coupling strengths, which is instead our goal—this can be achieved by evolution under a gradient. Consider, for example, the XY Hamiltonian  $\mathcal{H}_{XY} = \sum_{ij} b_{ij} (S_i^x S_j^x + S_i^y S_j^y)$ . Evolution under the propagator  $U(t, \tau) = e^{-i\mathcal{H}_z \tau} e^{-i\mathcal{H}_{XY} \tau} e^{i\mathcal{H}_z \tau}$ , where  $\mathcal{H}_z = \sum_i \omega_i S_i^z$  is obtained by a gradient, is equivalent to evolution under the Hamiltonian

$$\mathcal{H}'_{XY} = \sum_{ij} b_{ij} [(S_i^x S_j^x + S_i^y S_j^y) \cos(\delta\omega_{ij}\tau) + (S_i^x S_j^y - S_i^y S_j^x) \sin(\delta\omega_{ij}\tau)], \quad (1)$$

where  $\delta\omega_{ij} = \omega_j - \omega_i$ . The modulation is repeated to obtain  $U_0 = \prod_h U(t_h, \tau_h) \approx e^{i\tilde{\mathcal{H}}T}$  over the total time  $T$ , where the effective Hamiltonian  $\tilde{\mathcal{H}}$  can be approximated by a first order expansion. Given a desired target Hamiltonian  $\mathcal{H}_d = \sum_{ij} d_{ij}^1 (S_i^x S_j^x + S_i^y S_j^y) + d_{ij}^2 (S_i^x S_j^y - S_i^y S_j^x)$ , we obtain a set of equations in the unknowns  $\{t_h, \tau_h\}$  by imposing  $\tilde{\mathcal{H}} = \mathcal{H}_d$ .

To simplify the search for the correct timings, we can first apply a filter that cancels all unwanted couplings and use the equations above to only determine parameters for the remaining couplings. The filter is obtained by a dynamical implementation of a Bragg grating: we evolve under  $N$  cycles (while reducing the times to  $t_h/N$ ) with a gradient modulation  $U = \prod_{k=0}^{N-1} (e^{i\mathcal{H}_z \tau k} U_0 e^{-i\mathcal{H}_z \tau k})$  that weights the couplings by a factor  $\mathcal{G}_{ij}$ , with

$$\mathcal{G}_{ij} = \sum_{k=0}^{N-1} e^{ik\tau\delta\omega_{ij}} = e^{i(N-1)\tau\delta\omega_{ij}/2} \frac{\sin(N\tau\delta\omega_{ij}/2)}{\sin(\tau\delta\omega_{ij}/2)}. \quad (2)$$

We now make these ideas more concrete by considering a specific example, the engineering of an Hamiltonian that allows perfect QIT in mixed-state spin chains [30–33].

*Filtered engineering for QIT.*—For lossless transport, the simplest  $n$ -spin chain consists of nearest-neighbor (NN)

couplings that vary as  $d_j = d\sqrt{j(n-j)}$  [26], ensuring perfect transport at  $T = \pi/(2d)$ . Manufacturing chains with this precise coupling topology is a challenge due to fabrication constraints and the intrinsic presence of long-range interactions. Regular spin networks are instead found ubiquitously in nature: our method can be used to dynamically engineer the optimal Hamiltonian in these complex spin networks. Consider a dipolar-coupled spin network with Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{int}} + \mathcal{H}_z = \sum_{ik} b_{ik} (3S_i^z S_k^z - S_i \cdot S_k) + \sum_i \omega_i S_i^z, \quad (3)$$

where a magnetic-field gradient achieves the spatial frequency “tagging.” The target Hamiltonian for QIT in a  $n$ -spin chain is  $\mathcal{H}_d = \sum_{i=1}^{n-1} d_i (S_i^x S_{i+1}^x - S_i^y S_{i+1}^y)$ . We consider this interaction, instead of the more common XY Hamiltonian, since it drives the same transport evolution [34] and the double-quantum (DQ) Hamiltonian  $\mathcal{H}_{\text{DQ}} = \sum_{i<k} b_{ik} (S_i^x S_k^x - S_i^y S_k^y)$  can be obtained from the dipolar Hamiltonian via a well-known multiple-pulse sequence [27,28]. The sequence cancels the term  $\mathcal{H}_z$  and, importantly, allows time-reversal by a simple phase shift of the pulses. We can further achieve evolution under the field gradient only,  $\mathcal{H}_z$ , by using homonuclear decoupling sequences, such as WAHUA [18,19] or magic echo [35]. Thus, prior to applying the filtered engineering scheme, we use collective pulses to create the needed interactions  $\mathcal{H}_{\text{DQ}}$  and  $\mathcal{H}_z$ .

The filtered engineering sequence (e.g., Fig. 2) consists of alternating periods ( $\tau_j$ ) of free evolution under  $\mathcal{H}_z$  and double-quantum excitation  $\mathcal{H}_{\text{DQ}}$  (mixing periods  $\mathbf{t}_m$ ). We analyze the dynamics using average Hamiltonian theory [18,19]. Consider for simplicity a sequence with only two mixing and free evolution periods. Then, setting  $U_z(\tau) = e^{i\tau\mathcal{H}_z}$  and  $U_{\text{DQ}}(t) = e^{it\mathcal{H}_{\text{DQ}}}$ , the propagator for  $N$  cycles is  $U_N = [U_z(\tau_1)U_{\text{DQ}}(t_1/N)U_z(\tau_2)U_{\text{DQ}}(t_2/N)]^N$ , or

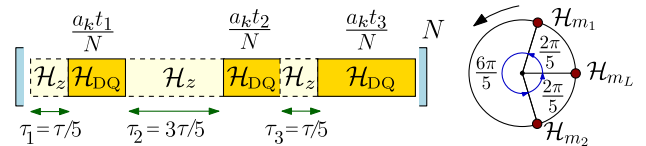


FIG. 2 (color online). Filtered engineering sequence, consisting of periods ( $\tau_j$ ) of free evolution under the gradient  $\mathcal{H}_z$  and mixing evolution under  $\mathcal{H}_{\text{DQ}}$  of duration  $t_j/N$ . The blocks are applied left to right, and the cycle is repeated  $N$  times. The sequence can be apodized by an appropriate choice of coefficients  $a_k$  at the  $k$ th cycle. Left: Example sequence for engineering transport in a five-spin chain in the complex network of Fig. 1. Explicit values of  $\mathbf{t}_m = \{t_1, t_2, \dots\}$  are in [27] and  $\tau = \pi/\omega$ . Right: Phasor representation [27] of Hamiltonian engineering. In the circle, we show the phases  $\phi_j = b_{i,i+1} t_j$  acquired by the  $S_i^+ S_{i+1}^+$  term of the toggling frame Hamiltonians  $\mathcal{H}_{m_j}$ .

$$U_N = \left[ U_z(N\tau) U_{\text{DQ}} \left( \frac{t_2}{N} \right) U_z^\dagger(N\tau) \right] \cdots \\ \times \left[ U_z(\tau) U_{\text{DQ}} \left( \frac{t_2}{N} \right) U_z^\dagger(\tau) \right] \left[ U_z(\tau_1) U_{\text{DQ}} \left( \frac{t_1}{N} \right) U_z^\dagger(\tau_1) \right], \quad (4)$$

where  $\tau = \tau_1 + \tau_2$ . Now,  $U_z(\tau) U_{\text{DQ}}(t) U_z^\dagger(\tau) = e^{it\mathcal{H}_m(\tau)}$ , where  $\mathcal{H}_m(\tau) = \sum_{i < k} b_{ik} (S_i^+ S_k^+ e^{i\tau\delta_{ik}} + S_i^- S_k^- e^{-i\tau\delta_{ik}})$  is the toggling frame Hamiltonian with  $\delta_{ik} = \omega_i + \omega_k$ . Employing the Suzuki-Trotter approximation [15],  $U_N$  is equivalent to evolution under the effective Hamiltonian

$$\bar{\mathcal{H}} = \sum_{i < j} \frac{b_{ij}}{NT} S_i^+ S_j^+ (t_1 e^{i\tau_1 \delta_{ij}} + t_2 e^{i(\tau_1 + \tau_2) \delta_{ij}}) \mathcal{G}_{ij} + \text{H.c.}, \quad (5)$$

with  $\mathcal{G}_{ij} = e^{i(N-1)\tau\delta_{ij}/2} \frac{\sin(N\tau\delta_{ij}/2)}{\sin(\tau\delta_{ij}/2)}$  and  $T = \sum_k t_k$ .

In general, for a sequence of free times  $\tau_z = \{\tau_1, \dots, \tau_L\}$  and mixing times  $\mathbf{t}_m = \{t_1, \dots, t_L\}$ , the average Hamiltonian is  $\bar{\mathcal{H}} = \sum_{i < j} S_i^+ S_j^+ F_{ij}(\tau_z, \mathbf{t}_m) \mathcal{G}_{ij}(\tau) + \text{H.c.}$ , where  $\tau = \sum_{j=1}^L \tau_j$  and we define the weighting function

$$F_{ij}(\tau_z, \mathbf{t}_m) = \frac{b_{ij}}{NT} \sum_k t_k \exp\left(i\delta_{ij} \sum_{h=1}^k \tau_h\right). \quad (6)$$

The grating  $\mathcal{G}_{ij}$  forms a sharp filter with maxima at  $\tau\delta_{ij} = 2m\pi$ . A linear 1D magnetic-field gradient along a selected chain of spins in the larger network sets the  $j$ th spin frequency to  $\omega_j = j\omega - \omega_0$ , where  $\omega_0$  is the excitation frequency. Each spin pair acquires a spatial phase under the gradient: if  $\omega\tau = \pi$  and  $2\omega_0\tau = 3\pi - 2m\pi$ , the NN couplings are preserved, while the next-nearest-neighbor couplings lie at the minima of the grating and are canceled (Fig. 3). Other non-NN, off-chain couplings lie at the grating side lobes and have greatly reduced amplitudes at large  $N$ .

Following the filter, the weighting function  $F_{j(j+1)}$  is constructed to yield the ideal couplings for perfect

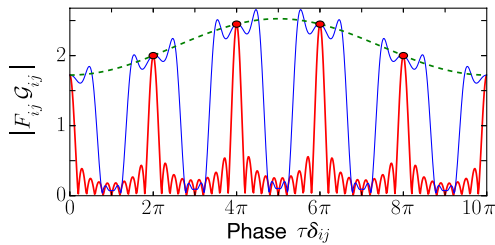


FIG. 3 (color online). Engineering filter function  $|F_{ij}\mathcal{G}_{ij}|$  for a five-spin chain, as a function of the phase  $\tau\delta_{ij}$ . A single cycle creates the weighting function  $F_{ij}$  (dashed line), which is transformed to sharp (red) peaks at the ideal couplings (circles) at a larger cycle number (here,  $N = 10$ ). The peak widths can be altered by apodization, e.g., sinc apodization (blue line)  $a_k = \sin[W(k - N/2)]/W(k - N/2)$ , with  $W = (\pi + 1)/2$  and normalized so that  $\sum_{k=1}^N a_k = N$ .

transport. We have a set of  $2n$  equations (for an  $n$ -spin chain)

$$\sum_{h=1}^L \sin\left[\omega(2j+1) \sum_{k=1}^h \tau_k\right] t_h b_{j,j+1} = 0, \quad \forall j \\ \sum_{h=1}^L \cos\left[\omega(2j+1) \sum_{k=1}^h \tau_k\right] t_h b_{j,j+1} \propto d_j, \quad \forall j, \quad (7)$$

with  $2L$  unknowns for  $L$  time steps. The number of conditions (thus of time steps) can be reduced by exploiting symmetry properties. For example, a gradient symmetric with respect to the chain center would automatically satisfy most of the conditions in Eq. (7) and only  $L = \lceil n/2 \rceil$  time steps would be required. Unfortunately, this solution is practical only for some chain lengths [27]; we thus focus on a suboptimal, but simpler, solution. Consider an odd  $n$ -spin chain. To enforce the mirror symmetry of  $d_j$  and ensure that the average Hamiltonian remains in DQ form, we impose time mirror symmetry  $t_j = t_{L-j}$ , while the gradient times are  $\tau_j/\tau = 3/n$  for  $j = (L+1)/2$  and  $\tau_j/\tau = 1/n$  otherwise (Fig. 2). This choice yields a linear system of equations for  $L = n - 2$  mixing periods  $\mathbf{t}_m$

$$F_{j(j+1)} \mathcal{G}_{j(j+1)} = \sum_k t_k \cos\left(\frac{2j\pi k}{n}\right) = d\sqrt{j(n-j)}. \quad (8)$$

Analogous solutions can be derived for even spin chains. A phasor representation [36] of how the evolution periods exploit the symmetries is presented in Fig. 2 and [27].

The tuning action of  $F_{j(j+1)} \mathcal{G}_{j(j+1)}$  is very rapid, achieving perfect fidelity  $f = \text{Tr}\{US_1^z U^\dagger S_n^z\}/2^n$  in just a few cycles. Increasing  $N$  reduces the error in the Trotter expansion by improving  $F_{j(j+1)}$  [Fig. 4(a)] as well as the selectivity of  $\mathcal{G}_{j(j+1)}$  [Fig. 4(b)]. The grating peak width decreases as  $2\pi/N$  [8], improving its selectivity linearly with  $N$  [27]. As shown in Fig. 4, about  $n$  cycles are required for almost perfect decoupling of the unwanted interactions ( $f > 0.95$ ).

The highly selective grating also avoids the need to isolate the chain and for the surrounding network to have

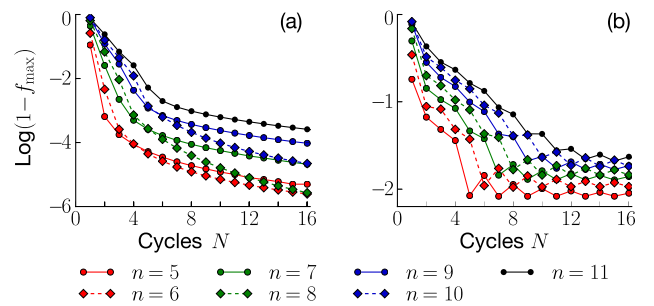


FIG. 4 (color online). Minimum transport infidelity obtained by filtered engineering, as a function of cycle number  $N$  for a  $n$ -spin dipolar chain with (a) NN couplings only and (b) all couplings.



a regular structure. However, in the presence of disorder in the chain couplings, one needs to compromise between broader grating peaks (via small  $N$ ) and poorer decoupling of unwanted interactions (Fig. 5). To improve the robustness of our scheme, we can further modulate the mixing times  $t_m$  by coefficients  $a_k$ ; this imposes an apodization of the grating function as  $\mathcal{G}_{ij} = \sum a_k e^{ik\tau\delta_{ij}}$ . Apodization can counter the disorder and dephasing that destroy the exact phase relationships among spins that enabled our Hamiltonian engineering method. The grating peaks can be made wider by a factor  $W$  (Fig. 3), and any coupling that is in phase to within  $W$  can still be engineered robustly (Fig. 6) at the expense of a poorer decoupling efficiency of long-range couplings. Apodization has other applications: for instance, it could be used to engineer nonlinear spin chains in lattices or, quite generally, to select any regular array of spins from a complex network—allowing a wide applicability of our method to many natural spin networks and crystal lattices [27].

*Approximation validity.*—The control sequence is designed to engineer the average Hamiltonian  $\mathcal{H}$  only to first order. Higher order terms arising from the Trotter expansion yield errors scaling as  $\mathcal{O}(t_k t_{k+1}/N^2)$ . Consider, e.g., the propagator for a five-spin chain

$$U_N = [e^{i(t_L/N)\mathcal{H}_{DQ}} e^{i(t_1/N)\mathcal{H}_m(\tau_1+\tau_2)} e^{i(t_1/N)\mathcal{H}_m(\tau_1)}]^N, \quad (9)$$

where  $\tau_1 = \pi/(5\omega)$  and  $\tau_2 = 3\pi/(5\omega)$ . This yields the desired  $\mathcal{H}$  with an error  $\mathcal{O}(t_1^2/N^2)$  for the first product and  $\mathcal{O}(2t_1 t_L/N^2)$  for the second. While increasing  $N$  improves the approximation, at the expense of larger overhead times, even small  $N$  achieves remarkably good fidelities, since, by construction,  $t_j \ll t_L \approx T$ . In essence, the system evolves under the unmodulated DQ Hamiltonian during  $t_L$ , yielding the average coupling strength, while the  $t_j$  periods apply small corrections required to reach the ideal couplings. Symmetrizing the control sequence would lead to a more accurate average Hamiltonian because of vanishing higher orders [37]. However, this comes at the cost of longer overhead times  $\tau_z$ ; thus, using a larger number of the unsymmetrized sequence is often a better strategy.

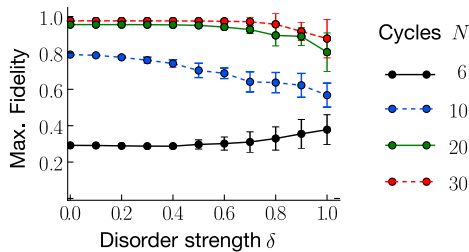


FIG. 5 (color online). Variation of maximum fidelity with disorder in the network (Fig. 1) surrounding the spin chain. The spins are displaced by  $\delta r$ , where  $r$  is uniformly distributed on  $[-r_0/2, r_0/2]$  (averaged over 30 realizations), with  $r_0$  the NN chain spin separation.

*Experimental viability.*—We consider an experimental implementation and show that high fidelity QIT at room temperature is achievable with current technology.

We assume that a spin lattice of NN separation  $r_0$ , yielding a NN coupling strength  $b = ((\mu_0\hbar)/4\pi)(\gamma^2/r_0^3)$ . If an ideal  $n$ -spin chain could be fabricated with maximum coupling strength  $b$ , the transport time would be  $T_{\text{id}} = (n\pi/8b)$  [30]. Alternatively, perfect state transfer could be ensured in the weak-coupling regime [31,33], with a transport time  $T_{\text{weak}} \approx (\Gamma\pi/b)$ , where  $\Gamma \gg 1$  ensures that the end spins are weakly coupled to the bulk spins. We compare  $T_{\text{id}}$  and  $T_{\text{weak}}$  to the time required for  $N$  cycles of the engineering sequence  $T_{\text{eng}}$ . Since  $t_L \gg t_j$ , to a good approximation, the total mixing time is  $t_L \leq \sum_j \sqrt{j(n-j)/(nb)} \approx \pi n/8b$ . Adding the overhead time  $N\tau$ , which depends on the available gradient strength as  $\tau = \pi/\omega$ , we have  $T_{\text{eng}} = (n\pi^2/16b) + (N\pi/\omega)$ . Since we can take  $\Gamma \approx n$  for the weak regime [31] and  $N \approx n$  for filtered engineering, a gradient larger than the NN coupling strength would achieve faster transport.

For concreteness, consider a crystal of fluorapatite  $[\text{Ca}_5(\text{PO}_4)_3\text{F}]$  that has been studied for quantum transport [38,39]. The  $^{19}\text{F}$  nuclear spins form parallel linear chains along the  $c$  axis, with intrachain spacing  $r_0 = 0.344$  nm ( $b = 1.29$  kHz), while the interchain coupling is  $\approx 40$  times weaker. Maxwell field coils [40] can generate sufficient gradient strengths, such as a gradient of  $5.588 \times 10^8$  G/m over a  $1$  mm<sup>3</sup> region [41], corresponding to  $\omega = 0.7705$  kHz. Far stronger gradients are routinely used in magnetic resonance force microscopy; for example, dysprosium magnetic tips [42] yield gradients of 60 G/nm, linear over distances exceeding 30 nm, yielding  $\omega = 82.73$  kHz. Setting  $\omega = 25$  kHz would allow  $\pi/2$ -pulse widths of about  $0.5$   $\mu\text{s}$  to have sufficient bandwidth to control chains exceeding  $n = 50$  spins. Homonuclear decoupling sequences [19,35] can increase the coherence time up to  $T_{\text{eng}}$ . Evolution under the DQ Hamiltonian has been shown to last for about 1.5 ms [43] in fluorapatite; decoupling during the  $U_z$  periods could increase this to 15 ms [35]. While pulse errors might limit the performance

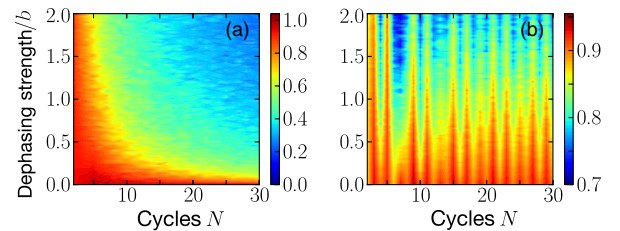


FIG. 6 (color online). Transport fidelity for a five-spin chain with dipolar couplings (NN coupling strength  $b$ ). The spins are subject to dephasing noise, modeled by an Ornstein-Uhlenbeck process of correlation time  $\tau_c = 2/b$  and strength  $2b$ , averaged over 100 realizations. (a) No apodization. (b) With sinc apodization [ $W = (\pi + 1)/2$ , as in Fig. 3].

of Hamiltonian engineering, there exist several methods to reduce these errors [44]. With  $\omega = 25$  kHz and 30 cycles, nearly lossless transport should be possible for a 25-spin chain.

Filtered Hamiltonian engineering could as well be implemented in other physical systems, such as trapped ions [13] or dipolar molecules [45] and atoms [16] in optical lattices. For instance, Rydberg atoms in optical lattices [46,47] could enable simulations at low temperature, thanks to the availability of long-range couplings and the ability to tune the lattice to create gradients. The scheme could also be extended to more complex 2D and 3D lattices [27].

*Conclusion.*—We have described a method for quantum simulation that does not require local control but relies on the construction of time-domain filter and weighting functions via evolution under a gradient field. The method achieves the engineering of individual spin-spin couplings starting from a regular, naturally occurring Hamiltonian. We presented a specific application to engineer spin chains for perfect transport, isolating them from a large, complex network. We showed that robust and high fidelity quantum transport can be driven in these engineered networks, with only experimental feasible control.

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