where $theta', \omega \ll 1$, a state that includes contributions from $n \pm 1$. This can done using the control methods in Step (4).

Step (4)– Hamiltonian evolution: This step of the algorithm is the simulation of the Hamiltonian H_p. We will begin by discussing the controls used for manipulating spins in NMR and then describe the simulation of the Hamiltonian.

In the rotating frame, the NMR system has a "drift" Hamiltonian (H_0 in Eq. (1))

$$H_{\mathrm{NMR}} = \sum_{l=1}^{N} \frac{\omega_l}{2} \sigma_l^z + \sum_{l=1}^{N-1} J_l \sigma_l^z \sigma_{l+1}^z. \tag{4}$$

The controls available in NMR experiments are rotations around the x and y axes for each individual qubit (represented by the spin of the nucleus) which have Hamiltonians of the form

$$F = \sum_{l=1}^{N} (u_l^x \sigma_l^x + u_l^y \sigma_l^y),$$

where the u_l^x, u_l^y are controllable (i.e., time-dependent as in Eq. (1). On the other hand, the Hamiltonians in Eq. (4) are always present. A powerful method that allows us to deal with such constraints (that are not unique to NMR) is *recoupling* (e.g., [52]).The idea is based on elementary angular momentum theory. We define $C_A^{\varphi} \circ e^{i\theta B} \equiv e^{i\varphi A} e^{i\theta B} e^{-i\varphi A}$, where A, B are generators of $su(2)$ (e.g., two Pauli matrices), and/or $\{A, B\} = 0$ while $A^2 = \mathbf{1}$. This *recoupling sequence* can be interpreted as the application of time-reversed pulses ($e^{\pm i\varphi A}$) before and after periods of free evolution $e^{i\theta B}$. Special cases of interest are (i) $C_A^{\pi/2} \circ e^{i\theta B} = e^{-i\theta B}$, (ii) $C_A^{\pi/4} \circ e^{i\theta B} = e^{i\theta(iBA)}$. Thus, to obtain evolution under $\frac{\omega_l}{2}\sigma_l^z$ we apply the (unoptimized) recoupling sequence $\exp(-\frac{i\omega_l}{2}\sigma_l^z t) = (e^{-iH_{\mathrm{NMR}}t/4} T_l e^{-iH_{\mathrm{NMR}}t/4} T_l')^2$, where $T_l = \otimes_{j \neq l} \sigma_j^x$, $T_l' = \otimes_{j \neq l}' \sigma_j^x$ where the prime indicates that j is even (odd) if l is even (odd). This takes $3N$ pulses. Similarly, we can evolve under any term $\sigma_j^z \sigma_{j+1}^z$ using $\sim 7N$ recoupling steps.

Next, we need to show how to simulate *long-range* interactions using H_{NMR} and F. The set $\{X_{lm} \equiv \frac{1}{2}(\sigma_l^x \sigma_m^x + \sigma_l^y \sigma_m^y), Y_{lm} \equiv \frac{1}{2}(\sigma_l^y \sigma_m^x - \sigma_l^x \sigma_m^y), Z_{lm} \equiv \frac{1}{2}(\sigma_l^z - \sigma_m^z)\}$ forms an $su(2)$ algebra, and commutes with $\sigma_m^z + \sigma_l^z$ for any l, m [53]. Thus $C_{X_{ll+1}}^{\pi/2} \circ Z_{l,l+1} = -Z_{l,l+1}$, while $C_{X_{ll+1}}^{\pi/2} \circ (\sigma_l^z + \sigma_{l+1}^z) = (\sigma_l^z + \sigma_{l+1}^z)$. Adding yields $C_{X_{ll+1}}^{\pi/2} \circ (\sigma_{l-1}^z \sigma_l^z) = \sigma_{l-1}^z \sigma_{l+1}^z$, so that $C_{X_{ll+1}}^{\pi/2} \circ e^{i\theta\sigma_{l-1}^z\sigma_l^z} = e^{i\theta\sigma_{l-1}^z\sigma_{l+1}^z}$. Thus $C_{X_{ll+1}}^{\pi/2}$ acts as a nearest-neighbor exchange operator. In order to implement $C_{X_{ll+1}}^{\pi/2}$ using H_{NMR} and F note that:

$$e^{-i\frac{\pi}{2}X_{ll+1}} = C_{\sigma_l^x+\sigma_{l+1}^x}^{-\pi/4} \circ e^{-i\frac{\pi}{4}\sigma_l^z\sigma_{l+1}^z} C_{\sigma_l^y+\sigma_{l+1}^y}^{\pi/4} \circ e^{-i\frac{\pi}{4}\sigma_l^z\sigma_{l+1}^z}.$$

It is simple to check that to create all possible couplings $\sigma_l^z \sigma_m^z$ in this manner requires $O(N^3)$ steps. This procedure allows us to use the short-range NMR Hamiltonian to simulate $J_l \sigma_l^z \sigma_m^z$ with $|l - m|$ arbitrary. Let us now show how to turn this into a simulation of $H_I \equiv \frac{1}{2}\sum_{l>m=1}^{N} V_{ml}(\sigma_m^x \sigma_l^x + \sigma_m^y \sigma_l^y)$. Suppose that H_{p} evolves for time τ. We can turn on $-J_l \sigma_l^z \sigma_m^z$ for a time τ_{ml} such that $2J_l\tau_{ml} = |V_{ml}|\tau$ (for a BCS Hamiltonian $V_{ml} < 0$). Doing this for all couplings separately (in series) shows

that the evolution operator $U^z(\tau) = \exp(-\frac{i}{2}\sum_{l>m} V_{lm}\sigma_l^z\sigma_m^z\tau)$ is obtained using the same $O(N^3)$ steps. By adjusting single-qubit operation times, we can implement $U^\alpha = \exp(i\frac{\pi}{4}\sum_l \sigma_l^\alpha)$, to yield: $\exp(-iH_I\tau) = \left(U^{x\dagger}U^z(\tau)U^x\right)\left(U^yU^z(\tau)U^{y\dagger}\right)$, using $O(N^3)$ steps. However, H_p also contains the term $H_0 \equiv \sum_{l=1}^N \frac{\varepsilon_l}{2}\sigma_l^z$, which does not commute with H_I. Clearly, by turning on single qubit NMR σ_l^z terms for times τ_l so that $\omega_l\tau_l = \varepsilon_l\tau$, we can simulate H_0 directly using N steps. The non-commutativity implies that we need a short-time approximation in order to simulate the full $U_\mathrm{p}(\tau) = \exp(-iH_\mathrm{p}\tau)$:

$$U_\mathrm{p}(\tau) = e^{-iH_0\tau}e^{-iH_I\tau} + O(\tau^2). \tag{5}$$

When the additional recoupling steps needed to turn off unwanted interactions (which we ignored above) are taken into account, using the method of [54], we find that $U_\mathrm{p}(\tau)$ requires a total of $s(N) = -\frac{4}{3}N^2 + \frac{32}{3}N - \frac{47}{3}N^3 + \frac{28}{3}N^4$ steps. This result may be improved somewhat if parallel operations are allowed. If H_NMR contains beyond-nearest-neighbor interactions then at most $O(N^5)$ steps are needed. The effect of the $O(\tau^2)$ errors in quantum algorithms due to the short-time approximation has been analyzed, e.g., in [15,16] By concatenating short-time evolution segments one can then obtain the finite time ($k\tau = t$) evolution operator $U_\mathrm{p}(t) \approx (U_\mathrm{p}(\tau))^k$ [6], in a total of $k\,s(N)$ steps.

Step (5)– Measurement: In NMR one measures the free-induction-decay (FID) signal, given by $V_\alpha(t) \propto \mathrm{Tr}(\rho(t)\sigma_\alpha^+)$, where $\rho(t)$ is the system density matrix and α is the index of the measured spin (qubit) [49]. Combining steps (ii)-(iv), we have $\rho(t) = U_\mathrm{p}(t)|\psi(0)\rangle\langle\psi(0)|U_\mathrm{p}^\dagger(t)$. To relate $V_\alpha(t)$ to the spectrum of the pairing Hamiltonian we introduce an appropriate basis. A complete set of conserved quantum numbers are the number of Cooper pairs n (= the number of 1's in a computational basis state, lowered by σ_α^-), the energy $E_{n,i}$ for fixed n, and a state degeneracy index β_i. Thus our basis states are labeled by $|n,i,\beta_i\rangle$ and $\rho(t)$ can be expanded as $\sum B_{n,i,\beta_i}B^*_{m,j,\beta_j}|n,i,\beta_i\rangle e^{i(E_{m,j}-E_{n,i})t}\langle m,j,\beta_j|$ with $|\psi(0)\rangle = \sum_{n,i,\beta_i} B_{n,i,\beta_i}|n,i,\beta_i\rangle$. We have

$$V_\alpha(t) \propto \sum_{m,n}\sum_{i,j} C^{(\alpha)}_{m,j;n,i}e^{i(E_{m,j}-E_{n,i})t}, \tag{6}$$

where $C^{(\alpha)}_{m,j;n,i} \equiv \sum_{\beta_i\beta_j} B_{n,i,\beta_i}B^*_{m,j,\beta_j}\langle m,j,\beta_j|\sigma_\alpha^-|n,i,\beta_i\rangle \propto \delta_{m,n-1}$. Fourier transforming, we obtain the energy spectrum $S(\omega) = \sum_{n,i,j}\tilde{C}^{(\alpha)}_{n-1,j;n,i}\delta(\omega - (E_{n-1,j} - E_{n,i}))$, with the gap defined as $2\Delta_n \equiv E_{n,1} - E_{n,0}$. Ideally, Δ_n can be found from a few runs with different initial n. There are two complications in practice: (i) Finding Δ_n in this manner depends on the coefficients $\tilde{C}^{(\alpha)}_{n-1,j;n,i}$ not vanishing. By measuring all qubits α, it is likely that sufficiently many non-zero coefficients will be available. (ii) The sharpness of the δ functions depends on how densely the signal $V_\alpha(t)$ is sampled. To resolve the gap, we will need to sample with a resolution $\Delta\omega = 2\pi/T < \Delta_n$. Recall that H_BCS conserves n. Thus the number of τ-intervals required for fixed n is $k(n) \gg \pi/(\tau\Delta_n)$, which is just the adiabatic condition again. A total of $\frac{1}{2}k(n)^2$ elementary evolutions steps, each simulating evolution under H_p for length τ, will thus be needed to simulate $\{U_\mathrm{p}(k\tau)\}_{k=1}^{T/\tau}$, and each such step takes $s(N)$ logic gates. The longest single run takes $k(n)s(N)$ steps, while $\frac{1}{2}k(n)^2s(N)$ is the total run-time of the algorithm. if the algorithm is to succeed in the absence

of error correction, then we must have $k(n)s(N) < T_2/\tau_{\rm logic}$, the ratio of decoherence to logic gate time. For NMR, $T_2/\tau_{\rm logic}$ can be $\sim 10^5$. To estimate $k(n)$ we need τ and Δ_n. The gap can be estimated experimentally, for nuclear and BCS systems using material dependent parameters [44,45,54]. Recall that τ is related to the short-time approximation which allowed us to neglect commutator terms in the expansion of $U_{\rm ad}(t)$. Since $e^{(A+B)\tau} \approx e^{A\tau}e^{B\tau}e^{-\frac{1}{2}[A,B]\tau^2}$, we need to estimate when $|[A,B]\tau| \ll \min(|A|,|B|)$. To obtain a rough estimate we consider a reduced BCS model [55]:$V_{ml} \equiv -V < 0$, $\varepsilon_l = \varepsilon_0 + ld$. In the BCS case the level spacing $d \ll V$, but $\varepsilon_0 \gg V$. Letting $A = \varepsilon_l \sigma_l^z$, $B = VX_{lm}$, we have $|[A,B]| = |V(\varepsilon_l - \varepsilon_m)Y_{lm}| > Vd$, while $\min(|A|,|B|) = V$. Thus the short-time approximation is valid when $\tau \ll 1/d$. Using $k(n) \gg \pi/(\tau\Delta_n)$ and $s(N) \approx 9N^4$ we thus have $k(n)\,s(N) \gg 30\frac{d}{\Delta_n}N^4$. In the BCS case $d/\Delta_n \ll 1$. Assuming $d/\Delta_n = 0.1$ we find $k(n)\,s(10) \gg 3 \times 10^4$, so that a simulation with $N \leq 10$ qubits seems to be within the reach of present day NMR simulations [49].

4. CONCLUSIONS

The Hamiltonian in Eq. (2) could represent several different physical systems and we have shown how to simulate a particular case, the BCS Hamiltonian, on an NMR quantum computing device. The same techniques could be applied to simulate the more general pairing Hamiltonians. The use of quasi-adiabatic evolution avoids the problem of determining the entire spectrum of the system, which could be inefficient. The algorithm scales as N^5, that is, the number of pulses grows as the fifth power of the number of qubits including the decoupling pulses required to "turn off" the interactions which are always present. Although this is a computationally efficient algorithm, it is still quite difficult to implement on present-day NMR apparatus. However, there are two present lines of research that show promise that these simulations may be useful for near-future non-trivial quantum simulations: present-day experiments and improved pulse sequences for NMR transformations.

The recent progress toward actual simulations has been quite promising. Several simulations have been carried out. Harmonic and an-Harmonic oscillations have been simulated [56].Three-body [57]and many-body type interactions have been simulated [58] and a BCS-type Hamiltonian, which was a modified version of the algorithm presented here, has been performed [59].

More efficient and/or accurate pulse sequences could improve the prospects for the various quantum simulations. Recent work has shown that very accurate gate sequences can be created [60-62]. Time-optimal control theory applied to NMR systems has been used to find pulses which improve many of the standard controls of the past [63-66].

Recalling that a fully scalable quantum computing device is not required to produce relevant simulations, along with the previously mentioned advances in experiment and theory of quantum simulation, we believe there is ample evidence that quantum simulations will soon provide advances in physics and the related sciences.

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