

Reducing Constraints on Quantum Computer Design by Encoded Selective Recoupling

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The requirement of performing both single-qubit and two-qubit operations in the implementation of universal quantum logic often leads to very demanding constraints on quantum computer design. We show here how to eliminate the need for single-qubit operations in a large subset of quantum computer proposals: those governed by isotropic and XXZ , XY -type anisotropic exchange interactions. Our method employs an encoding of one logical qubit into two physical qubits, while logic operations are performed using an analogue of the NMR selective recoupling method.

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Most proposals for quantum computer (QC) design rely on the execution of both single-qubit and two-qubit operations. Typically these two types of operations involve rather different manipulations and constraints. This often leads to serious technical difficulties, a problem which has been recognized and addressed in the context of QC proposals with isotropic Heisenberg spin-exchange interactions [1,2], through the use of quantum codes [3–9]. It is important to note that isotropic exchange is an idealization which in reality is likely to be perturbed due to surface and interface effects, as well as spin-orbit coupling [10]. We focus here primarily on QC proposals that are governed by anisotropic exchange interactions [11–15] (the XXZ and XY models, defined below). These systems either share some of the difficulties in implementing single-qubit gates exhibited by Heisenberg systems [1,2] (e.g., in the case of the quantum Hall proposal [11], extreme g -factor engineering, highly localized and inhomogeneous magnetic fields, and heating due to the high-intensity rf field needed for single-spin operations), or have other problems resulting from the need to implement both single- and two-qubit gates. For example, in the quantum dots in cavities proposal [12] elimination of the single-qubit operations would halve the number of lasers, significantly simplifying the experimental setup. There is therefore a compelling motivation to reexamine the need for single-qubit operations in the execution of quantum logic. Here we show how the complications associated with single-qubit operations can be avoided through the use of NMR-like recoupling methods [16] applied to an encoding of two physical qubits into one logical qubit, which we developed in [17]. Our method allows universal quantum logic to be attained through switching on/off exchange interactions only, without requiring external single-qubit operations. The method requires a modest overhead in the number of physical qubits and gate operations, but this seems like a fair price to pay in return for the reduction in complexity of experimental setup. Through the use of recoupling we are able to unify the treatment of both isotropic and anisotropic exchange. Similar to [8,9] but

using less stringent methods, we show how to reduce the overhead in the encoding proposed earlier for the isotropic case [3–6] from three physical qubits per logical (encoded) qubit to two, under the assumption that the single-particle spectrum is nondegenerate. In the XXZ case, our implementation of the controlled-phase (CPHASE) gate uses as few as four interactions (in parallel mode on qubits arranged in 1D). The efficient encoding, and the small overhead in number of gate applications we report here, suggests that the hurdle of single-qubit operations may be overcome in forthcoming experiments implementing elementary quantum logic in isotropic or anisotropic condensed or gas phase systems [1,2,11–15].

Exchange Hamiltonians.—Using spin notation, the exchange interaction quite generally [18] has the form $H_{\text{ex}} = \sum_{\alpha=x,y,z} \sum_{i<j} J_{ij}^{\alpha} \sigma_i^{\alpha} \sigma_j^{\alpha}$, where σ_i^{α} are the Pauli matrices, and the summation is over all qubit pairs i, j . Tunability of the exchange constants J_{ij}^{α} is at the heart of all solid-state proposals, and has been studied in detail, e.g., in [1]. The isotropic (Heisenberg) case corresponds to $J_{ij}^{\alpha} \equiv J_{ij}$. The XY model is the case $J_{ij}^x = J_{ij}^y, J_{ij}^z = 0$. Examples of QC proposals that fall into this category are the quantum Hall proposal [11], quantum dots [12,13], and atoms in cavities [14]. The XXZ model is the case $J_{ij}^x = \pm J_{ij}^y \neq J_{ij}^z$. [We refer to $+$ ($-$) as the axially symmetric (antisymmetric) case.] When surface and interface effects are taken into account, the XY examples, as well as the Heisenberg examples [1,2], are better described by the axially symmetric XXZ model. Additional sources of nonzero J_{ij}^z in the XY examples can be second-order effects (e.g., virtual cavity-photon generation without spin flips in [12]). A natural XXZ example is that of electrons on helium [15]. All these QC proposals were originally supplemented with *external* single-qubit operations, which can be written as $F = \sum_i f_i^x \sigma_i^x + f_i^y \sigma_i^y$. As argued above, these operations almost invariably lead to various (system-specific) difficulties, so we will not assume that they are available. In general one must also consider the free Hamiltonian $H_0 = \sum_i \frac{1}{2} \varepsilon_i \sigma_i^z$, where ε_i is the single-particle spectrum. In general, this spectrum will be nondegenerate, e.g., due

TABLE I. Comparison of some QC proposals in terms of difficulty of implementing two-qubit (J_{ij}^α), internal (ε_i), and external single-qubit operations ($f_i^{x,y}$). $H_0 = \text{fixed}$ means that it is hard to independently change each ε_i .

System	Two-qubit Hamiltonian	$H_0 = \sum_i \frac{1}{2} \varepsilon_i \sigma_i^z$	External $f_i^{x,y}$
Spin-coupled quantum dots [1]	Heisenberg, controllable	Fixed	Hard
Donor atom nuclear/electron spins [2]	Heisenberg, controllable	Fixed	Hard
Quantum Hall [11]	XY , controllable	Fixed	Hard
Quantum dots/atoms in cavities [12,14]	XY , controllable	Controllable	Easy, requires additional lasers
Exciton-coupled quantum dots [13]	XY , controllable	Fixed	Hard
Electrons on helium [15]	XXZ , only J_{ij}^+ controllable	Controllable	Easy but slow and hard to tune

to different local g factors [1,2]. Which of the *internal* parameters $\{J_{ij}^\alpha, \varepsilon_i\}$ are controllable is a system-specific question, as summarized in Table I. We now proceed to show how to perform (encoded) universal quantum computation while respecting the constraints imposed upon controllability of $\{J_{ij}^\alpha, \varepsilon_i\}$ by the various systems.

Encoding and operations.—First, we rewrite the general exchange Hamiltonian in a form which emphasizes axial symmetry:

$$H_{\text{ex}} = \sum_{i < j} J_{ij}^- R_{ij}^x + J_{ij}^+ T_{ij}^x + J_{ij}^z \sigma_i^z \sigma_j^z, \quad (1)$$

where

$$T_{ij}^x = \frac{1}{2}(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y), \quad R_{ij}^x = \frac{1}{2}(\sigma_i^x \sigma_j^x - \sigma_i^y \sigma_j^y), \quad (2)$$

and $J_{ij}^\pm = J_{ij}^x \pm J_{ij}^y$. Thus, the axially symmetric (antisymmetric) case corresponds to $J_{ij}^- = 0$ ($J_{ij}^+ = 0$). Note that T_{ij}^x can also be written as $\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+$ [where $\sigma_i^\pm = (\sigma_i^x \pm i\sigma_i^y)/2$], i.e., resonant energy transfer between qubit pairs. An important example of this is the Förster process, whereby through a Coulomb interaction an exciton hops between neighboring quantum dots that are sufficiently close. This has been used to show that a variety of quantum information processing tasks, such as the preparation of entangled states of excitons, can be performed in coupled quantum dots [13]. Our results apply to this scenario as well. In the axially symmetric case, our code is simply $|0_L\rangle_m = |\uparrow\rangle_{2m-1} \otimes |\downarrow\rangle_{2m}$ and $|1_L\rangle_m = |\downarrow\rangle_{2m-1} \otimes |\uparrow\rangle_{2m}$ for the m th encoded qubit, $m = 1, \dots, N/2$. In the axially antisymmetric case, $|0_L\rangle = |\uparrow\uparrow\rangle$ and $|1_L\rangle = |\downarrow\downarrow\rangle$ (in simplified notation). Thus, logical qubits correspond to pairs of nearest neighbor physical qubits (e.g., spins). Preparation and measurement of these states was discussed in Ref. [17]. Briefly, preparation relies on relaxation to the ground state of the Hamiltonian T_{ij}^x (R_{ij}^x) in the axially symmetric (antisymmetric) case, while measurement (which can also be used for preparation) employs an analogue of Kane's ac capacitance scheme [2]. It is important to note that none of the terms in H_{ex} are capable of flipping spins i, j *separately*. Therefore the axially symmetric and antisymmetric subspaces are decoupled. This means that we can independently operate on the corresponding subspaces. Our discussion below is carried out in tandem for these two cases. With the single number m serving to label our encoded qubits, it is advantageous

to compactify our notation further. Let $J_m^\alpha \equiv J_{2m-1,2m}^\alpha$ ($\alpha = z, \pm$), and $\varepsilon_m^\pm \equiv (\varepsilon_{2m-1} \pm \varepsilon_{2m})/2$.

Let us now introduce operators which implement rotations on the encoded qubits. Let $T_m^x \equiv T_{2m-1,2m}^x$ and $T_m^z = \frac{1}{2}(\sigma_{2m-1}^z - \sigma_{2m}^z)$; $R_m^x \equiv R_{2m-1,2m}^x$ and $R_m^z = \frac{1}{2}(\sigma_{2m-1}^z + \sigma_{2m}^z)$, where $T_{2m-1,2m}^x$ and $R_{2m-1,2m}^x$ were defined in Eq. (2). As we showed in [17], T_m^x (R_m^x) acts as the Pauli σ^x matrix on the axially symmetric (antisymmetric) m th encoded qubit. Similarly, T_m^z (R_m^z) acts as σ^z . Therefore pairs of these operators each generate an “encoded $SU(2)$ ” group on the logical qubits, i.e., the group of all single-encoded-qubit operations. Moreover, $[T_m^\alpha, R_m^\beta] = 0$ (in agreement with the decoupling of the symmetric and antisymmetric subspaces), so that these single-encoded-qubit operations can be implemented in classical parallelism. Let us now momentarily assume that we have independent control over all parameters ($\varepsilon_m^\pm, J_{ij}^\pm, J_{ij}^z$). Below, we will relax this constraint by using selective recoupling. In order to implement single-encoded-qubit operations, we turn on the interactions J_m^\pm and the energy sums and differences ε_m^\pm , while leaving off the interactions between spins belonging to different encoded qubits (i.e., $J_{2m,2m+1}^\alpha = 0$), as well as leaving all J_{ij}^z off. We can then rewrite the total Hamiltonian $H = H_0 + H_{\text{ex}}$ as

$$H = \sum_{m=1}^{N/2} (\varepsilon_m^- T_m^z + J_m^+ T_m^x) + (\varepsilon_m^+ R_m^z + J_m^- R_m^x), \quad (3)$$

while omitting a constant term. Written in this form, it is clear that by selectively turning on/off the parameters ε_m^-, J_m^+ (ε_m^+, J_m^-) for the axially symmetric (antisymmetric) qubit, one can implement all single-encoded-qubit operations, by using Euler angle rotations to generate the encoded $SU(2)$ group. Moreover, H is expressed as a sum over terms acting on different encoded qubits, so that all $N/2$ encoded qubits (of a given symmetry) can be operated on independently. In other words, the encoded Hilbert space has a tensor product structure.

To complete the general discussion, we must also show how to couple different encoded qubits through a nontrivial (entangling) gate. For the XXZ model, this turns out to be even simpler than implementing single-encoded-qubit operations. Turning on the coupling $J_{2m,2m+1}^z$ between pairs of spins belonging to two neighboring encoded qubits immediately implements the encoded $-T_m^z T_{m+1}^z$ ($R_m^z R_{m+1}^z$) Hamiltonian on the axially symmetric (antisymmetric)

qubits. To see this, note that in the axially symmetric case, e.g., $|0_L\rangle_1|0_L\rangle_2 = |01\rangle_{12}|01\rangle_{34} \xrightarrow{\sigma_2^z \sigma_3^z} -|01\rangle_{12}|01\rangle_{34} = -|0_L\rangle_1|0_L\rangle_2$, and similarly for the other three combinations: $|0_L\rangle|1_L\rangle \rightarrow |0_L\rangle|1_L\rangle$, $|1_L\rangle|0_L\rangle \rightarrow |1_L\rangle|0_L\rangle$, $|1_L\rangle|1_L\rangle \rightarrow -|1_L\rangle|1_L\rangle$ so that in all $\sigma_2^z \sigma_3^z$ indeed acts as $-T_1^z T_2^z$. Since, as is well known [19], the CPHASE gate is directly obtainable by turning on the Hamiltonian $\sigma^z \otimes \sigma^z$ between physical qubits, in our case turning on $J_{2m,2m+1}^z$ yields a CPHASE gate between encoded qubits. We consider the XY model below, since it requires the introduction of the selective recoupling method. For the XXZ model, this encoded CPHASE together with the single-encoded-qubit operations suffice to perform encoded universal quantum computation [20].

Recoupling and encoding recoupling.—Recall that, as discussed above, in each instance of H_{ex} (Heisenberg, XY, XXZ) one typically has control over only one type of parameter out of the set $\{J_{ij}^\alpha, \varepsilon_i\}$. In our treatment above, we made liberal use of all parameters, and it is now time to relax this assumption. To show this, we now demonstrate how selective recoupling, applied to our encoded qubits, provides the requisite flexibility. Let us first briefly recall the basic idea of selective recoupling [16] through a simple NMR example. In a two-spin molecule in NMR, the internal Hamiltonian is $H_{\text{NMR}} = \sum_{i=1}^2 \varepsilon_i \sigma_i^z + J_{12}^z \sigma_1^z \sigma_2^z$ with uncontrollable parameters ε_i, J_{12}^z . However, control over ε_i is needed to implement z -axis rotations, while control over J_{12}^z is needed to implement a CPHASE. This is done by pulsing an external magnetic field along the x axis. Let A and B be anticommuting Hermitian operators where $A^2 = I$ (I is the identity matrix). Then the operation of “conjugating by A ,”

$$\begin{aligned} C_A \circ \exp(iB) &\equiv \exp(-iA\pi/2) \exp(iB) \exp(iA\pi/2) \\ &= \exp(-iB), \end{aligned} \quad (4)$$

causes B 's sign to be flipped. Thus, $\exp(-iH_{\text{NMR}}\tau) \times [C_{\sigma_1^x} \circ \exp(-iH_{\text{NMR}}\tau)] = \exp[-2i\tau\varepsilon_2\sigma_2^z]$, which implements a rotation through an angle $\theta = 2\tau\varepsilon_2$ about the z axis of the second spin. Notably, the Ising coupling term $\sigma_1^z \sigma_2^z$ has been eliminated. A similar calculation reveals that $\exp(-iH_{\text{NMR}}\tau)[C_{\sigma_2^z} \circ C_{\sigma_1^x} \circ \exp(-iH_{\text{NMR}}\tau)] = \exp[-2i\tau J_{12}^z \sigma_1^z \sigma_2^z]$, i.e., the selective implementation of the Ising coupling term through an angle τJ_{12}^z . Notice that to achieve this effect all that was needed was control over the parameters turning on/off the σ_i^x terms. Physically, the reason that H_{NMR} was neglected during the $\pi/2$ rotations is that typically in NMR the σ_i^x terms can be made much larger than H_{NMR} . Selective recoupling methods can be extended to deal with any number of spins coupled through an NMR-type Hamiltonian, and efficient methods using Hadamard matrices have been developed for both homonuclear [21] and heteronuclear systems [22,23].

Consider now an XXZ-type Hamiltonian where the J_m^+ parameters are controllable but ε_m^- and J_m^z are fixed. As argued above, this is a model of the XY examples

of QC proposals [11–14] that takes certain symmetry-breaking mechanisms into account. We can now map the selective recoupling method directly onto our problem. For simplicity, let us consider just the axially symmetric case. Then we can rewrite $H = H_0 + H_{\text{ex}}$ as $H_{\text{AX}} = \sum_{m=1}^{N/2} \varepsilon_m^- T_m^z - J_m^z T_m^z T_{m+1}^z + J_m^+ T_m^x$, where we have omitted a constant term. The important point is now that T_m^x and T_m^z satisfy the properties required of A and B above, *on the code subspace*. In fact, the structure of H_{AX} is exactly analogous to that of H_{NMR} , the only difference being that the T operators act on encoded qubits as opposed to directly on physical spins. Hence, the argument that held for H_{NMR} holds here as well: By using recoupling through “conjugation by T_m^x ” we can selectively turn on and off the single-encoded-qubit rotation T_m^z and the encoded-Ising interaction $T_m^z T_{m+1}^z$. This example of “encoded selective recoupling” establishes that encoded universal computation in the XXZ model can be done using control over the J_m^+ parameters alone.

Next, consider the XY model, i.e., the idealized version of the proposals in [11–14], with controllable J_{ij}^+ , but fixed ε_i . We still use the encoding $|0_L\rangle = |\uparrow\uparrow\rangle, |1_L\rangle = |\downarrow\downarrow\rangle$. To implement encoded single-qubit operations, we can use the same encoded recoupling method as for the XXZ model. As for encoded two-qubit operations, we now no longer have the $\sigma_i^z \sigma_j^z$ terms. Since the XY model with nearest neighbor interactions can be shown not to be universal [17], we turn on also next-nearest neighbor J_{ij}^+ terms (these can still be nearest neighbor in a 2D hexagonal geometry). First note that $C_{T_{12}^x} \circ T_{23}^x = i\sigma_1^z \sigma_2^z T_{13}^x$. Now assume we can control J_{13}^+ ; then, using conjugation by $\pi/4$, $C_{\frac{1}{2}T_{13}^x} \circ (C_{T_{12}^x} \circ T_{23}^x) = \sigma_2^z (\sigma_3^z - \sigma_1^z)/2$. Since $\sigma_1^z \sigma_2^z$ is constant on the code subspace it can be ignored. On the other hand, $\sigma_2^z \sigma_3^z$ again acts as $-T_1^z T_2^z$, i.e., as an encoded $\sigma^z \otimes \sigma^z$. This establishes universal encoded computation in the XY model.

Cost.—Let us now count how many elementary steps are needed to implement the various quantum computing primitives in the XXZ model. We define such a step as a single pulse whereby a single J_{ij}^α is switched on and then off. We will assume only the least demanding architecture of nearest neighbor interactions and a 1D layout of spins. Improvements are certainly possible with next-nearest neighbor interactions and/or a 2D geometry. For single-encoded-qubit operations, it takes one step to turn on a rotation about the encoded x axis (under the standard assumption that we can make $|J_m^+| \gg |\varepsilon_m^-|, |J_m^z|$), while it takes four steps to implement a rotation about the encoded z axis (turn on T_m^x for $\pi/2$, free evolution under $\varepsilon_m^- T_m^z - J_m^z T_m^z T_{m+1}^z$, repeat with T_m^x for $-\pi/2$). Therefore using the standard Euler angle construction it takes at most six steps to implement any single-encoded-qubit rotation. The encoded CPHASE operation is similar: If we assume that T_m^x and T_{m+1}^x can be turned on in parallel, then the same count of four steps as for encoded z axis rotations applies; otherwise we need to add two more operations, for

a total of six steps. In the XY case the implementation of CPHASE given above takes five steps.

Encoded recoupling for the Heisenberg case.— Elimination of single-qubit operations in the isotropic exchange case was first shown in [3], and further developed in [4–6]. With a fully degenerate H_0 this required encoding one qubit into three. We now show how to simplify this encoding, assuming a nondegenerate H_0 . Our code is the same as for the axially symmetric case above, and the same as that used in [8,9], but our method is less stringent. Reference [8] used spin-resonance techniques, with the rather demanding requirement that the spin-spin interaction strength be modulated at high frequency. Reference [9] showed how universal computation can be performed by varying the strength of the exchange coupling using nonoscillatory pulses. This scheme is very much in the spirit of our solution, but it has the problem of undesired spin rotations taking place while the interaction is off. We solve this problem here using the selective recoupling method. Let us write the total Hamiltonian as $H = H_0 + H_{\text{Heis}}$, where $H_{\text{Heis}} = \sum_{i<j} J_{ij}(T_{ij}^x + \frac{1}{2}\sigma_i^z \sigma_j^z)$ with $\frac{1}{2}J_{ij}^+ = J_{ij}^x = J_{ij}^y = J_{ij}^z = J_{ij}$. The exchange coupling parameters J_{ij} are assumed to be controllable, while H_0 is not (except by application of a global magnetic field). Therefore, similar to the anisotropic case, when we turn on $J_m \equiv J_{2m-1,2m}$ the Hamiltonian can be written as $H_{\text{Heis}} = \sum_{m=1}^{N/2} (\epsilon_m^- T_m^z + J_m T_m^x) + \Delta$, where $\Delta = \sum_{m=1}^{N/2} (\epsilon_m^+ R_m^z + \frac{J_m}{2} \sigma_{2m-1}^z \sigma_{2m}^z)$ acts trivially on the code space and, hence, can be omitted. By recoupling using T_m^x , we can selectively turn on and off the single-encoded-qubit rotation T_m^z , as above, thus generating the encoded- $SU(2)$ group only on the desired encoded qubit. Next, let us show how to selectively turn on a two-qubit Hamiltonian such as $T_1^z T_2^z = \sigma_2^z \sigma_3^z$. If we directly turn on $h_{23} = J_{23} \sum_{\alpha=x,y,z} \sigma_2^\alpha \sigma_3^\alpha$, the encoded space will leak. Recoupling can extract the $\sigma_2^z \sigma_3^z$ term as follows. First, note that $C_{T_1^x} \circ e^{-i\pi T_1^z/2} = e^{i\pi T_1^x/2}$, and $C_{T_1^z} \circ h_{23} = J_{23}(-\sigma_2^x \sigma_3^x - \sigma_2^y \sigma_3^y + \sigma_2^z \sigma_3^z)$. Hence, $e^{-ih_{23}t/2} C_{T_1^z} \circ e^{-ih_{23}t/2} = e^{-iJ_{23}\sigma_2^z \sigma_3^z t}$, so that $T_1^z T_2^z$ may be implemented selectively using six steps, which completes the requirements for universal computation. It is interesting to contrast these results with the 19 steps required in serial mode for the analogous operation in the isotropic case, assuming fully degenerate H_0 (seven steps are required in parallel mode in 2D) [6]. As a final comment, note that the code we used here is a decoherence-free subspace (DFS) and thus offers automatic protection against collective dephasing errors [4], as recently demonstrated in an ion trap experiment [24]. When other errors are present, one may use the method of concatenating DFSs with quantum error correcting codes [25], at the price of introducing greater qubit overhead, or use a combination of recoupling and decoupling techniques [26].

Conclusions.—The requirement of performing both single- and two-qubit operations in one quantum comput-

ing device often leads to severe technical constraints and difficulties. We have shown here that selective recoupling, as applied to encoded qubits, is a very general method to overcome these problems. It allows all quantum logic operations to be performed by turning on/off pairwise exchange interactions. The trade-off is modest: A qubit is encoded into the state of two neighboring spins, and universal quantum logic gates require only 4–6 interactions to be turned on/off in a simple 1D geometry with nearest neighbor coupling. We believe that this alternative to the hard requirements of quantum computing with single-qubit gates may substantially simplify the design of quantum computers.

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