Quantum Computing with Spin Cluster Qubits

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(Received 17 June 2002; published 27 January 2003)

We study the low energy states of finite spin chains with isotropic (Heisenberg) and anisotropic (*XY* and Ising-like) antiferromagnetic exchange interaction with uniform and nonuniform coupling constants. We show that for an odd number of sites a spin cluster qubit can be defined in terms of the ground state doublet. This qubit is remarkably insensitive to the placement and coupling anisotropy of spins within the cluster. One- and two-qubit quantum gates can be generated by magnetic fields and intercluster exchange, and leakage during quantum gate operation is small. Spin cluster qubits inherit the long decoherence times and short gate operation times of single spins. Control of single spins is hence not necessary for the realization of universal quantum gates.

DOI: 10.1103/PhysRevLett.90.047901 PACS numbers: 03.67.Lx, 75.10.Jm

Quantum computers outperform classical computers on certain tasks [1–4]. The main challenge on the way to a universal quantum computer is to achieve control over single quantum mechanical two state systems (qubits) while preserving long decoherence times. Electron [5,6] and nuclear [7,8] spins have been identified as promising candidates for qubits because they are natural two state systems and decoherence times for the spin degree of freedom are unusually large [9,10].

For both electron [5] and nuclear spin [8] qubits, one-qubit gates can be realized by local magnetic fields or by electrically tuning a single spin into resonance with an oscillating field. Two-qubit gates rely on electrical control of the exchange interaction between neighboring electron spins. However, even for electrons in quantum dots with a typical diameter of 50 nm, the required local control over electrical and magnetic fields is challenging. One possibility to circumvent the problem of either local magnetic fields [11] or local exchange interaction [12] is to encode the qubit in several spins. Such encoding has also been studied in the context of coherence-preserving qubits [13]. However, all these schemes still require control at the single-spin level.

More generally, the requirements on both local magnetic and electrical fields can be relaxed by increasing the size of the qubit. In the present work, we show that, for a wide class of antiferromagnetic spin $s = 1/2$ chains with an odd number of sites n_c,

$$\hat{H} = \sum_{i=1}^{n_c-1} f_i[J_\perp(\hat{s}_{i,x}\hat{s}_{i+1,x} + \hat{s}_{i,y}\hat{s}_{i+1,y}) + J_z\hat{s}_{i,z}\hat{s}_{i+1,z}], \quad (1)$$

the ground state doublet of the array [Fig. 1(a)] can define a new "spin cluster qubit" for which quantum gate operation times and decoherence rates increase only moderately with array size. These features are surprisingly stable with respect to anisotropy ($J_\perp \neq J_z$) and spatial variation (described by f_i) of the intracluster exchange, the spatial shape of the fields controlling quantum gate operation, and the cluster dimension. Spin cluster qubits can be realized in a wide variety of systems, e.g., arrays of quantum dots [5,14], clusters of P atoms in a Si matrix [8], and electron spins in molecular magnets. In contrast to the encoded qubits suggested in earlier work [11–13], quantum computation with spin cluster qubits is possible without control over local spin interactions.

Isotropic spin chains as qubits.—For illustration, we first discuss a spin chain with isotropic uniform exchange, $J_\perp = J_z > 0$ and $f_i \equiv 1$ in Eq. (1). Energy eigenstates can be labeled according to their quantum numbers of total spin $\hat{\mathbf{S}} = \sum_{i=1}^{n_c} \hat{\mathbf{s}}_i$ and the z component of total spin, $\hat{S}_z$. Because of the antiferromagnetic exchange, states in which the total spin of the chain is minimized are energetically most favorable [15]. For odd n_c, the ground state is a $S = 1/2$ doublet separated from the next excited state by a gap $\Delta \sim J\pi^2/2n_c$ determined by the lower bound of the des Cloiseaux-Pearson spectrum. We define the spin cluster qubit in terms of the $S = 1/2$ ground state doublet by $\hat{S}_z|0\rangle = (\hbar/2)|0\rangle$ and $\hat{S}_z|1\rangle = -(\hbar/2)|1\rangle$. The states $\{|0\rangle, |1\rangle\}$ do not, in general, have a simple representation in the single-spin product basis, but rather are superpositions of $n_c!/[(n_c - 1)/2]![(n_c + 1)/2]!$ states [Fig. 1(b)]. For example, for the simplest nontrivial spin cluster qubit with $n_c = 3$,

$$|0\rangle = \frac{2}{\sqrt{6}}|\uparrow\rangle_1|\downarrow\rangle_2|\uparrow\rangle_3 - \frac{1}{\sqrt{6}}|\uparrow\rangle_1|\uparrow\rangle_2|\downarrow\rangle_3 - \frac{1}{\sqrt{6}}|\downarrow\rangle_1|\uparrow\rangle_2|\uparrow\rangle_3, \quad (2)$$

and $|1\rangle$ is obtained by flipping all spins.

In spite of their complicated representation in the single-spin product basis, $|0\rangle$ and $|1\rangle$ are in many respects

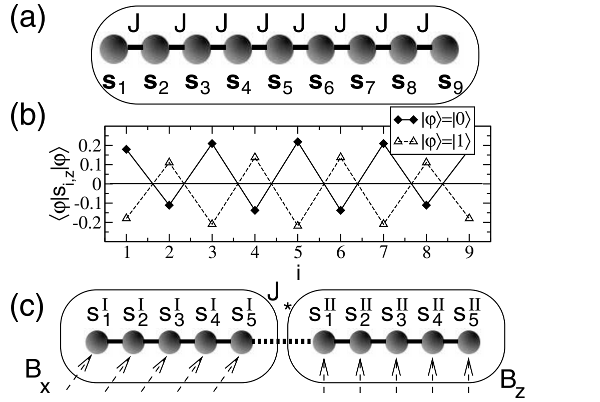

FIG. 1. (a) The states of the spin cluster [Eq. (1)] define the spin cluster qubit. (b) $|0\rangle$ and $|1\rangle$ have a complicated representation in the single-spin product basis, as evidenced by the local spin density. (c) Quantum gates are generated by magnetic fields or g-factor engineering (one-qubit gates) and a switchable interqubit exchange $J_*(t)$ (two-qubit gates).

very similar to the states $|\uparrow\rangle$ and $|\downarrow\rangle$ of a single spin and, hence, can be used as qubit states for universal quantum computing [5]. Because $\{|0\rangle, |1\rangle\}$ belong to one $S = 1/2$ doublet such that $\hat{S}^-|0\rangle = \hbar|1\rangle$, and $\hat{S}^+|1\rangle = \hbar|0\rangle$ where $\hat{S}^\pm = \hat{S}_x \pm i\hat{S}_y$, a magnetic field $\mathbf{B}$ constant over the cluster acts on the spin cluster qubit in the same way as on a single-spin qubit. Hence, both the one-qubit phase shift and the one-qubit rotation gate can be generated by magnetic fields $B_z(t)$ and $B_x(t)$, respectively, possibly in combination with g-factor engineering [5,16]. For a given $B_{z,x}(t)$, operation times of one-qubit gates are equal to the ones for the single-spin qubit. We note that, due to quantum mechanical selection rules, we have $\langle i|\hat{\mathbf{S}}|0\rangle = \langle i|\hat{\mathbf{S}}|1\rangle = 0$ for $|i\rangle \neq |0\rangle, |1\rangle$, i.e., a uniform magnetic field does not cause leakage to states outside the ground state doublet.

For the CNOT gate, one requires a tunable exchange interaction $\hat{H}_*$ between one or several spins of neighboring spin cluster qubits I and II. For simplicity, we first restrict our attention to an isotropic exchange coupling $\hat{H}_* = J_*(t)\hat{\mathbf{s}}^{\rm I}_{n_c} \cdot \hat{\mathbf{s}}^{\rm II}_1$ between the outermost spins of clusters I and II, respectively [Fig. 1(c)]. This exchange interaction will, in general, not only couple states within the two-qubit basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, but will also lead to transitions to excited states (leakage). If $J_*(t)$ changes adiabatically, i.e., on time scales long compared to $\hbar/\Delta$ and $|J_*(t)| \ll \Delta$ for all times t, leakage remains small (see below). The action of $\hat{H}_*$ can then be described by an effective Hamiltonian in the two-qubit product basis

$$\hat{H}_* = J_{*z}(t)\hat{S}^{\rm I}_z\hat{S}^{\rm II}_z + \frac{J_{*\perp}(t)}{2}(\hat{S}^{\rm I+}\hat{S}^{\rm II-} + \hat{S}^{\rm I-}\hat{S}^{\rm II+}), \quad (3)$$

where the roman numbers label the spin clusters, $J_{*z}(t) = 4J_*(t)|_{\rm I}\langle 0|\hat{s}^{\rm I}_{n_c,z}|0\rangle_{\rm I}||_{\rm II}\langle 0|\hat{s}^{\rm II}_{1,z}|0\rangle_{\rm II}|$, and $J_{*\perp}(t) = 4J_*(t)|_{\rm I}\langle 1|\hat{s}^{\rm I}_{n_c,x}|0\rangle_{\rm I}||_{\rm II}\langle 0|\hat{s}^{\rm II}_{1,x}|1\rangle_{\rm II}|$. We have shown that the coupling $\hat{H}_*$ is isotropic also in the two-qubit product basis and acts on the states $|0\rangle$ and $|1\rangle$ of neighboring spin chains in the same way as an isotropic exchange between two single spins. $|_{\rm I}\langle 1|\hat{s}^{\rm I}_{n_c,x}|0\rangle_{\rm I}|$ and $|_{\rm II}\langle 0|\hat{s}^{\rm II}_{1,x}|1\rangle_{\rm II}|$ determine the gate operation time $\tau_{\rm CN}$ of the CNOT gate, $|i\rangle|j\rangle \to |i\rangle|i + j \bmod 2\rangle$ where $i, j = 0, 1$. For $n_c = 9, \ldots, 15$, the matrix elements are of order 0.1, i.e., a factor of 5 smaller than for a single spin 1/2.

Although we have so far discussed one-qubit gate operations induced from spatially uniform magnetic fields, such uniformity may be difficult to achieve experimentally. One-qubit gates can be performed with spatially varying fields $B_{i,x}$ and $B_{i,z}$ (or g factors) for which $|\langle 1|\sum_{i=1}^{n_c} g_i\mu_B B_{i,x}\hat{s}_{i,x}|0\rangle| \neq 0$ and $\langle 0|\sum_{i=1}^{n_c} g_i\mu_B B_{i,z}\hat{s}_{i,z}|0\rangle \neq 0$, respectively. Similarly, the analysis leading to Eq. (3) remains valid for a wide class of coupling Hamiltonians $\hat{H}_*$ for which $\langle 10|\hat{H}_*|01\rangle \neq 0$. For illustration we discuss two examples. First, couplings between several spins of cluster I to several spins of cluster II, such as $\hat{H}_* = J_*\sum_{i=1}^{n_c}\hat{\mathbf{s}}^{\rm I}_i \cdot \hat{\mathbf{s}}^{\rm II}_i$, are permitted and even lead to a decrease of $\tau_{\rm CN}$ because the coupling of several spins in the microscopic Hamiltonian leads to an increased effective coupling between the clusters. Second, a modification of the intracluster exchange couplings by $\hat{H}_*$ due to additional terms such as $J_*\hat{\mathbf{s}}^{\rm II}_1 \cdot \hat{\mathbf{s}}^{\rm II}_2$ does not invalidate the proposed gate operation scheme. This illustrates the most significant advantage of the spin cluster qubits over single-spin qubits—that *it is sufficient to control magnetic fields and exchange interactions on a scale of the spin cluster diameter.* For the linear spin cluster qubit, this length scale is n_c times larger than the original qubit.

A set of universal quantum gates is necessary but not sufficient for the realization of a quantum computer. Rather, additional requirements must be met, including initialization, decoherence times large compared to gate operation times, and readout [17]. Initialization can be achieved by cooling in a magnetic field B_z to a temperature [5] $T \lesssim g\mu_B B_z/k_B < \Delta/k_B$. Because the state of the spin cluster qubit, $|0\rangle$ or $|1\rangle$, determines the sign of the local magnetization at each site within the spin chain [Fig. 1(b)], readout of the spin cluster qubit can be accomplished by readout of the spins within the cluster [5,18].

An important consideration is the effect of decoherence on spin cluster qubits. The scaling of the decoherence rate with system size depends on the microscopic decoherence mechanism. For electron spins in quantum dots, fluctuating fields and nuclear spins have been identified as dominant sources [5,6,19]. We model [5] the action of fluctuating magnetic fields by $\hat{H}^B_\phi = b(t)\hat{S}_z$ where $b(t)$ is Gaussian white noise, $\langle b(t)b(0)\rangle = 2\pi\gamma^B\delta(t)$. Because the magnetic moment $\pm g\mu_B/2$ of the spin cluster qubit is the same as for a single spin, the decoherence rate [20] $\pi\gamma^B$ is independent of n_c. In contrast, the decoherence rate due to fluctuating fields acting independently on each site increases linearly with n_c.

Spin dynamics during gate operation.—One- and two-qubit gates induce spin dynamics in the clusters, and leakage out of the ground state doublet is required to remain small. In order to quantify leakage, by numerical integration of the Schrödinger equation we trace the time evolution of a small spin cluster qubit ($n_c = 5$) during the one-qubit rotation gate. The qubit is rotated coherently from $|0\rangle$ into $|1\rangle$, which corresponds to a simultaneous rotation of all spins [Figs. 2(a) and 2(b)]. The one-qubit rotation can also be generated by an inhomogeneous field B_x acting, e.g., only on the central spin of the cluster as long as $g\mu_B B_x \ll \Delta$ [Figs. 2(a) and 2(b)]. Leakage due to instantaneous switching is less than 0.3% for $g\mu_B B_x = 0.1J$, but increases with $g\mu_B B_x$ [Fig. 2(b)].

For the special cases $J_{*z} = J_{*\perp}$ and $J_{*z} = 0$ in Eq. (3), an explicit pulse sequence for the CNOT gate has been derived previously in Refs. [5,21]. We define the unitary time evolution operator $U_*(\pi/2) = T\exp(-i\int dt\hat{H}_*/\hbar)$, with $-\int dt J_{*\perp}(t)/\hbar = \pi/2$. Then, more generally,

$$U_{\rm CNOT} \sim e^{-i\pi S_y^{\rm II}/2} e^{i2\pi \mathbf{n}_1\cdot\mathbf{S}^{\rm I}/3} e^{i2\pi\mathbf{n}_2\cdot\mathbf{S}^{\rm II}/3} U_*(\pi/2) \times e^{i\pi S_y^{\rm I}} U_*(\pi/2) e^{-i\pi S_x^{\rm I}/2} e^{-i\pi S_x^{\rm II}/2} e^{i\pi S_y^{\rm II}/2} \quad (4)$$

is the CNOT gate for an arbitrary effective XXZ-coupling Hamiltonian [Eq. (3)] if $J_{*\perp} \neq 0$, where $\mathbf{n}_1 = (1, -1, 1)/\sqrt{3}$ and $\mathbf{n}_2 = (1, 1, -1)/\sqrt{3}$. We confirmed that for the complete pulse sequence the dynamics of two spin clusters is as predicted on the basis of the two-level description (Fig. 3). Leakage induced by $\hat{H}_*$ is small for $J_* \ll \Delta$ because all spins in the clusters corotate, although $\hat{H}_*$ couples only the outermost spins.

Spatially varying and anisotropic exchange.—We show next that spin cluster qubits are extremely robust with respect to spatial variation [accounted for by f_i in Eq. (1)] and anisotropies ($J_\perp \neq J_z$) of the intracluster exchange. For spatially varying isotropic exchange ($J_\perp = J_z = J$), the system still exhibits a $S = 1/2$ ground state doublet [15] and the above analysis remains valid. In systems such as quantum dot arrays where it is possible to engineer the intracluster exchange Jf_i during sample growth, the qubit basis states $\{|0\rangle, |1\rangle\}$ can be tailored to some extent.

We next consider the XY chain, $J_z = 0$. By the Jordan-Wigner transformation [22], the XY spin chain is mapped onto a system of noninteracting spinless fermions with spatially varying hopping amplitudes, $\hat{H} = -(J_\perp/2)\sum_{i=1}^{n_c-1} f_i(\hat{\psi}_{i+1}^\dagger\hat{\psi}_i + \hat{\psi}_i^\dagger\hat{\psi}_{i+1})$, where $\hat{\psi}_i$ annihilates a Jordan-Wigner fermion at site i. We find that the one-particle Hamiltonian has $(n_c - 1)/2$ states with negative and positive energy, respectively, which are pairwise related to each other by staggering of the wave function. There is one zero-energy eigenstate

$$e_0 \propto \left(1, 0, -\frac{f_1}{f_2}, 0, \frac{f_1 f_3}{f_2 f_4}, 0, \ldots, \pm\frac{f_1 f_3 \cdots f_{n_c-2}}{f_2 f_4 \cdots f_{n_c-1}}\right). \quad (5)$$

The ground state doublet of the XY chain corresponds to the lowest $(n_c - 1)/2$ and $(n_c + 1)/2$ Jordan-Wigner fermion levels filled. For $f_i \equiv 1$, $\Delta \simeq \pi J_\perp/n_c$. Similarly to the spin chain with isotropic exchange, one-qubit gates can be realized by magnetic fields $B_z(t)$ and $B_x(t)$ unless $\langle 1|\hat{S}_x|0\rangle = 0$. For $n_c \leq 9$ and $f_i \equiv 1$, $|\langle 1|\hat{S}_x|0\rangle| \geq 0.4$. From Eq. (5), one can also calculate all matrix elements entering Eq. (3). In particular, for $f_i \equiv 1$, $\langle 0|\hat{s}_{n_c,z}|0\rangle = 1/(n_c + 1)$ and $|\langle 1|\hat{s}_{n_c,x}|0\rangle| = 1/\sqrt{2(n_c + 1)}$. Because of the anisotropy of the intrachain exchange, $\hat{H}_*$ (which is isotropic in the single-spin operators) translates into an anisotropic effective Hamiltonian Eq. (3). Nevertheless, the CNOT gate can still be realized according to Eq. (4). For the anisotropic chain, a magnetic field applied along an axis $\mathbf{n}$ translates into a rotation around the axis $\propto (2|\langle 1|\hat{S}_x|0\rangle| n_x, 2|\langle 1|\hat{S}_x|0\rangle| n_y, n_z)$ in the Hilbert space spanned by $\{|0\rangle, |1\rangle\}$. A one-qubit rotation around an arbitrary axis hence requires

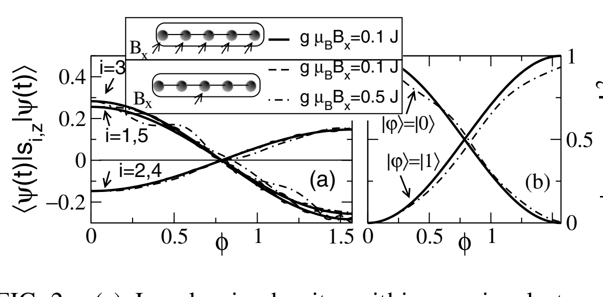

FIG. 2. (a) Local spin density within a spin cluster qubit ($n_c = 5$) as function of $\phi \propto g\mu_B B_x t/\hbar$ obtained by integration of the full Schrödinger equation for homogeneous (solid line) and inhomogeneous B_x (dashed and dashed-dotted lines). (b) For $B_x \ll \Delta/g\mu_B$ or homogeneous B_x, the state rotates coherently from $|0\rangle$ to $|1\rangle$. For a magnetic field acting only on the central spin of the cluster, the leakage increases to 7% for $g\mu_B B_x = 0.5J$.

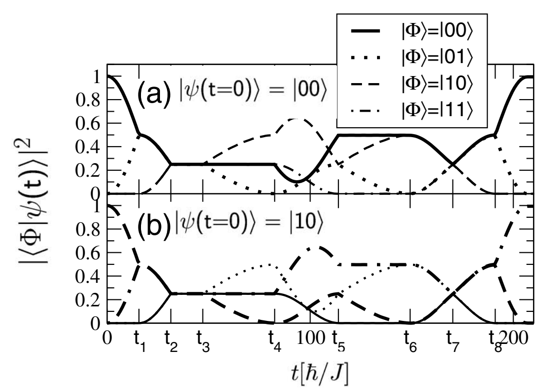

FIG. 3. CNOT gate for two small spin cluster qubits ($n_c = 3$) obtained by numerical integration of the Schrödinger equation [see Fig. 1(c)]. The plotted probabilities and the phases (not displayed) show that (a) $|00\rangle \rightarrow |00\rangle$ and (b) $|10\rangle \rightarrow |11\rangle$. We have chosen a pulse sequence [Eq. (4)] with instantaneous switching (at times t_i), $B = 0.1J/g\mu_B$, and $J_* = 0.1J$. Leakage due to instantaneous switching (0.7% for our parameters) can be reduced by decreasing J_* and B.

appropriate rescaling of **B**. For example, the rotation corresponding to $\exp(i2\pi \mathbf{n}_1 \cdot \mathbf{S}^{\mathrm{I}}/3)$ [Eq. (4)] for the isotropic chain can be achieved by applying a magnetic field $B = B_0[1 + 2/(2|\langle 1|\hat{S}_x|0\rangle|)^2]^{1/2}/\sqrt{3}$ along the axis $\propto (1, -1, 2|\langle 1|\hat{S}_x|0\rangle|)$ for a time $2\pi\hbar/3g\mu_B B_0$. For given J_* and B, the CNOT gate operation time increases at most linearly with n_c.

For $J_z \gg J_\perp$ (Ising-like systems), where $|0\rangle = |\uparrow\rangle_1|\downarrow\rangle_2 \ldots |\uparrow\rangle_{n_c} + \mathcal{O}(J_\perp/\mathrm{J}_z)$, the ground state doublet is separated from the next excited state by an n_c-independent $\Delta \sim J_z \min(f_i)$. In perturbation theory in $J_\perp/J_z$, for $f_i \equiv 1$, the matrix elements $|\langle 1|\hat{S}_x|0\rangle|$, $|\langle 1|\hat{s}_{n_c,x}|0\rangle| \sim (2J_\perp/J_z)^{(n_c-1)/2}$ decrease exponentially with n_c. Even for medium sized chains $n_c \gtrsim 9$ and $J_\perp/J_z < 0.2$, an isotropic $\hat{H}_*$ translates into an effective Ising Hamiltonian, $J_{*\perp} \simeq 0$ in Eq. (3). Hence, only quantum computing schemes which rely on Ising interactions [23] are feasible.

Discussion.—The main idea of the present work applies not only to spin chains but remains valid for a wide class of antiferromagnetic systems with uncompensated sublattices, also in higher dimensions $d > 1$ and for larger spins $s > 1/2$. We illustrate the advantages of spin cluster qubits for electron spins in quantum dots with a typical diameter of $d = 50$ nm, where the exchange coupling can be as large as 10 K [6]. One-qubit operations are realized, e.g., by g-factor engineering in the presence of a static field $B \simeq 1$ T. We now compare the performance of a spin cluster qubit formed by $n_c = 5$ quantum dots coupled by an intracluster exchange $J = 10$ K with a single-spin qubit. To obtain an estimate, we consider gate operation by switching the magnetic field B to $g\mu_B B = 0.7$ K, and $J_* = 2.3$ K [6], small compared to the energy gap $\Delta = 7.2$ K of the spin cluster. For single spins, the gate operation times for the NOT and CNOT gate are 36 and 117 ps, respectively. Assuming that the magnetic field decreases smoothly from its maximum value at the central spin of the spin cluster qubit to $0.2B$ acting on spins 2 and 4, we find that the operation time for one-qubit gates increases by a factor $1/2|\langle 1|\hat{s}_{3,x} + 0.2\hat{s}_{2,x} + 0.2\hat{s}_{4,x}|0\rangle| = 2.2$ compared to the single spin. Similarly, for the operation time of the CNOT gate we find 280 ps for the spin cluster qubit. The main advantage of the spin cluster qubit is that it is sufficient to control magnetic fields or g factors on a length scale of $n_c d = 250$ nm and exchange couplings on a scale of $2n_c d = 500$ nm. This would allow one to control the exchange between neighboring clusters optically [14] at the expense of an increase in gate operation times by a factor of 2.

Other possible applications for spin cluster qubits include, e.g., P atoms in a Si matrix [8] and molecular magnetic systems [24]. For electron spins of P atoms in a Si matrix, the requirement of positioning P with lattice spacing precision [8,25] can be circumvented by the use of spin clusters instead of single spins. More generally, the present work shows that for universal quantum gates control is not required at the level of single electron spins. Because a qubit can always be mapped onto a spin 1/2, the general principle of arranging several qubits into a cluster qubit applies to any quantum computing proposal.

This work was supported by the EU TMR network No. HPRN-CT-1999-00012 (F. M. and D. L.), DARPA SPINS and QuIST (J. L. and D. L.), the Swiss NCCR Nanoscience (D. L.), and the Swiss NSF (D. L.). We acknowledge discussions with G. Burkard, V. Cerletti, H. Gassmann, F. Marquardt, and P. Recher.

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