Environmentally decoupled *sds*-wave Josephson junctions for quantum computing

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Quantum computers have the potential to outperform their classical counterparts in a qualitative manner, as demonstrated by algorithms[1] which exploit the parallelism inherent in the time evolution of a quantum state. In quantum computers, the information is stored in arrays of quantum two-level systems (qubits), proposals for which include utilizing trapped atoms and photons[2–4], magnetic moments in molecules[5] and various solid-state implementations[6–10]. But the physical realization of qubits is challenging because useful quantum computers must overcome two conflicting difficulties: the computer must be scalable and controllable, yet remain almost completely detached from the environment during operation, in order to maximize the phase coherence time[11]. Here we report a concept for a solid-state 'quiet' qubit that can be efficiently decoupled from the environment. It is based on macroscopic quantum coherent states in a superconducting quantum interference loop. Our two-level system is naturally bistable, requiring no external bias: the two basis states are characterized by different macroscopic phase drops across a Josephson junction, which may be switched with minimal external contact.

Our Josephson junction utilizes unconventional superconductors with order-parameter symmetry lower than the symmetry of the underlying crystal lattice. Recent phase-sensitive experiments on $YBa_2Cu_3O_7$ single crystals have established the *d*-wave nature of the copper oxide materials, thus identifying unambiguously the first unconventional superconductor[12,13]. The sign change in the order parameter of these materials can be exploited to construct a new type of *s*-wave–*d*-wave–*s*-wave Josephson junctions exhibiting a degenerate ground state and a double-periodic current–phase characteristic. The basic idea is sketched in Fig. 1: connecting the positive (100) and negative (010) lobes of a *d*-wave superconductor with a *s*-wave material produces a π-loop with a current-carrying ground state characteristic of *d*-wave symmetry[12]. Here we use an alternative geometry and match the *s*-wave superconductors (*S* in Fig. 1) to the (110) boundaries of the *d*-wave (D) material. The usual Josephson coupling (proportional to $(1 - \cos\phi)$) vanishes for symmetry reasons and we arrive at a bistable device, where the leading term in the coupling takes the form $E_d \cos 2\phi$ with minima at $\phi = \pm\pi/2$ (here ϕ denotes the gauge-invariant phase drop across the junction and E_d is the coupling energy). In our design we need the minima at the positions $\phi = 0, \pi$—the necessary shift is achieved by going over to an asymmetric SDS′ junction with a large DS′ coupling (Fig. 1). The static DS′ junction shifts the minima of the active SD junction by the desired amount, $\pi/2$. A similar double-periodic junction was recently realized by combining two *d*-wave superconductors oriented at a 45° angle[14].

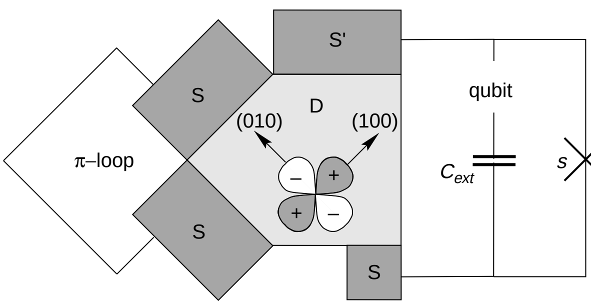

Figure 1 Schematic of the junction. Geometrical arrangements between *s*- and *d*-wave superconductors producing a π-loop (as in the phase-sensitive experiment by Wollman *et al.*[12]) and a qubit, basic building block of a quantum computer, are shown.

The ground states of our SDS′ junction are degenerate and carry no current, while still being distinguishable from one another: for example, after connecting the junction to a large inductance loop, the π state is easily identified through the induced current. It is this double-periodicity and the associated degeneracy in the ground state of the SDS′ which we want to exploit here for quantum computation: combining the SDS′ junction, a capacitor, and a conventional *s*-wave junction into a SDS′ SQUID loop, we construct a bistable element that satisfies all the requirements for a qubit, the basic building block of a quantum computer. (SQUID indicates a superconducting quantum interference device.) Below we give a detailed account of the operational features of our device.

Consider a small-inductance (L) SQUID loop with $I_J L \ll \Phi_0$, where I_J denotes the (Josephson) critical current of the loop and $\Phi_0 = hc/2e$ is the flux unit. Such a loop cannot trap magnetic flux ($\Phi = 0$) and the gauge-invariant phase differences ϕ_1 and ϕ_2 across the two junctions follow each other, as the uniqueness of the

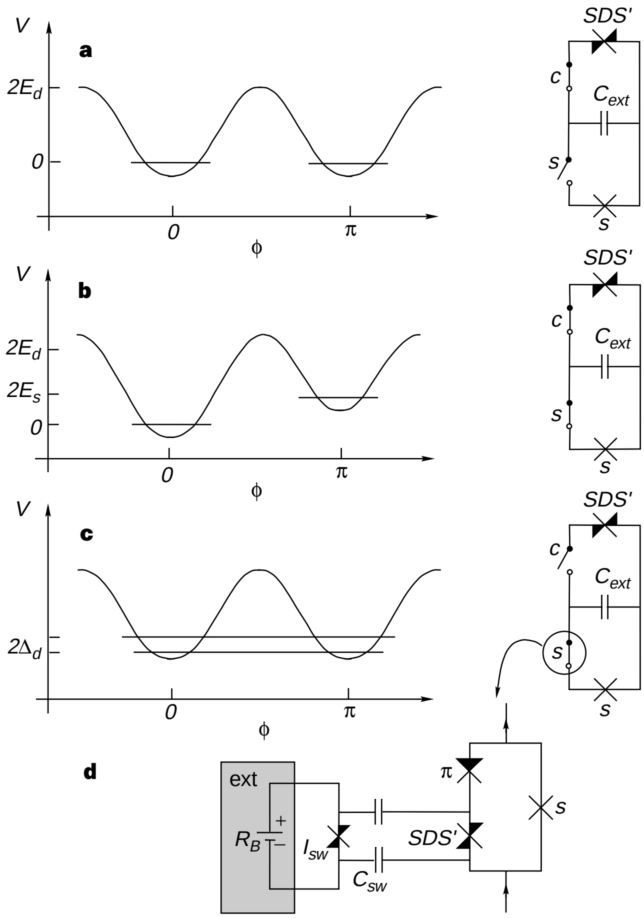

Figure 2 Energy–phase diagrams for the SDS′ SQUID loop. **a**, Idle-state: the switches are set to '*c* on' and '*s* off'–the relative dynamics are quenched, leaving the state unchanged. **b**, Phase-shifter: with the switch settings '*c* on' and '*s* on' the relative phase between $|0\rangle$ and $|\pi\rangle$ increases linearly with time. **c**, Amplitude-shifter: the switch setting '*c* off' isolates the *d*-wave junction. An initial state $|0\rangle$ oscillates back and forth between $|0\rangle$ and $|\pi\rangle$, allowing for a shift of amplitude. **d**, the SDS′ junction, a π junction, and a *s*-wave junction combined into a SQUID loop and serving as a switch.

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wavefunction requires that $\phi_1 - \phi_2 = 2\pi\Phi/\Phi_0$ (ref. 15). Combining an SDS′ junction with a coupling energy E_d and a conventional s-wave junction (coupling E_s) into an SDS′ SQUID loop, we obtain a potential energy

$$V(\phi) = E_d(1 - \cos 2\phi) + E_s(1 - \cos\phi) \quad (1)$$

exhibiting two minima at $\phi = 0, \pi$ (Fig. 2). The switch s allows us to manipulate their energy separation, choosing between minima which are either degenerate or separated by $2E_s$.

In the quantum case, the phase fluctuates as a consequence of the particle–phase duality[15]. The phase fluctuations are driven by the electrostatic energy required to move a Cooper pair across the junction, and are described by the kinetic energy $T(\dot\phi) = (\hbar/2e)^2 C\dot\phi^2/2$, where C denotes the loop capacitance. The dynamics of ϕ are manipulated by inserting a large switchable (by switch c) capacitance $C_{\rm ext}$ into the loop acting in parallel with the capacitances C_d and C_s of the d- and s-wave junctions. We note that the lagrangean $L = T - V$ of our loop is formally equivalent to that of a particle with 'mass' $m \propto C$ moving in the potential $V(\phi)$.

With the switch settings 'c on' 's off' (Fig. 2a), the loop capacitance is large and the junction exhibits a double degenerate ground state which we characterize via the phase coordinated ϕ, $|0\rangle$ and $|\pi\rangle$. Closing the switch s (Fig. 2b), the degeneracy is lifted and while $|0\rangle$ becomes the new ground state, the $|\pi\rangle$-state is shifted upwards by the energy $2E_s$ of the s-wave junction, the latter being frustrated (that is, pushed to maximal energy) when $\phi = \pi$. On the other hand, opening the switch c (Fig. 2c), completely isolates the d-wave junction and leads to the new ground and excited states $|\pm\rangle = [|0\rangle \pm |\pi\rangle]/\sqrt{2}$ separated by the tunnelling gap $2\Delta_d$. The latter relates to the barrier $2E_d$ and the capacitance C_d of the d-wave junction via[15] $\Delta_d \propto E_d \exp(-2\sqrt{C_d E_d/e^2})$. Closing the switch c, the capacitance is increased by $C_{\rm ext}$ and the tunnelling gap is exponentially suppressed. Using the above three settings, we can perform all the necessary single qubit operations, as follows.

Idle-state. The switch settings 'c-on' and 's-off' define the qubit's idle-state. While the large capacitance $C_{\rm ext}$ inhibits tunnelling, the degeneracy of $|0\rangle$ and $|\pi\rangle$ guarantees a parallel time evolution of the two states. This idle-state is superior to other designs, where the two states of the qubit have different energies and it is necessary to keep track of the relative phase accumulated between the basis states.

Phase shifter. Closing the switch s separates the energies of the basis states $|0\rangle$ and $|\pi\rangle$ by an amount $2E_s$. Using a spinor notation for the two-level system, the relative time evolution of the two states is described by the hamiltonian $H_s = -E_s\sigma_z$, with σ_z a Pauli matrix. Keeping the switch s on during the time t, the time evolution of the two states is given by the unitary rotation $u_z(\varphi) = \exp(-i\sigma_z\varphi/2)$ with $\varphi = -2E_s t/\hbar$.

Amplitude shifter. Assume we have prepared the loop in the ground state $|0\rangle$ and wish to produce a superposition by shifting some weight to the $|\pi\rangle$ state. Opening the switch c in the loop (Fig. 2c), the time evolution generated by the hamiltonian $H_d = \Delta_d\sigma_x$ of the open loop induces the rotation $u_x(\vartheta) = \exp(-i\sigma_x\vartheta/2)$ with $\vartheta = 2\Delta_d t/\hbar$. The system then oscillates back and forth between $|0\rangle$ and $|\pi\rangle$ with frequency $\omega = \Delta_d/\hbar$ and keeping the switch c open for an appropriate time interval t, we obtain the desired shift in amplitude (note that the qubit remains isolated from the environment during these Rabi oscillations).

Imposing the conditions $E_d \gg E_s, \Delta_d$ on the coupling energies, we make sure that the two states $|0\rangle$ and $|\pi\rangle$ are well defined while simultaneously involving only the low-energy states $|0\rangle$ and $|\pi\rangle$ of the system. Furthermore, all times involved should be smaller than the decoherence time $\tau_{\rm dec}$, requiring $E_s, \Delta_d \gg \hbar/\tau_{\rm dec}$.

The present set-up differs significantly from the conventional (large-inductance) SQUID loop design, where the low-lying states are distinguished via the different amount of trapped flux and their manipulation involves external magnetic fields or biasing currents. SQUID loops of this type are being used in the design of classical Josephson-junction computers[16] and have also been proposed[9] for the realization of quantum computers. However, this set-up suffers from the generic problem that the flux moving between the loops leads to a magnetic-field-mediated long-ranged interaction between the individual loops and also produces an unwanted coupling to the environment. By contrast, our device remains decoupled from the environment, the operating states do not involve currents, and switching between states can be triggered with a minimal contact to the external world—we therefore call our qubit implementation 'quiet'.

We now consider how to perform two-qubit operations within an array of SDS′ SQUID loops. A two-qubit state is a coherent superposition of single qubit states and can be expressed in the basis $\{|xy\rangle\}$, where $x, y \in \{0, \pi\}$ denote the phases on the d-wave junctions of the first (x) and second (y) qubit, respectively. Unitary operations acting on these states are represented as 4×4 unitary matrices. Single-qubit operations u acting on the second qubit take the block-matrix form

$$U_2 = \begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix} \quad (2)$$

and a similar block form selecting odd and even rows and columns defines the single-qubit operations on the first qubit. As all logic operations on two qubits can be constructed from combinations of single-qubit operations and the 'controlled-NOT' gate[1] it is sufficient to define the operational realization of the latter. The controlled-NOT gate performs the following action on the two qubits: with the first (controller) qubit in state $|x\rangle$ and the second (target qubit) in state $|y\rangle$ the operation shall leave the target qubit unchanged if $x = 0$, while flipping it between 0 and π when $x = \pi$, in matrix notation:

$$U_{\rm CNOT} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \sigma_x \end{pmatrix} \quad (3)$$

The above controlled-NOT operation can be constructed from the 2-qubit phase shifter. Connecting two individual qubits in their idle-state over a s-wave junction into a SQUID loop, the states $|00\rangle$ and $|\pi\pi\rangle$ become separated from the states $|0\pi\rangle$ and $|\pi0\rangle$ by the energy $2E_{s_b}$ of the s-wave junction. Keeping the two qubits connected during the time t introduces a phase shift $\chi = -2E_{s_b}t/\hbar$ between the two pairs of states:

$$U_{\rm ps}(\chi) = \begin{pmatrix} u_z(\chi) & 0 \\ 0 & u_z(-\chi) \end{pmatrix} \quad (4)$$

The controlled-NOT gate (equation (3)) then can be constructed from the phase-shifter (equation (4)) via the following sequence of single- and two-qubit operations (see ref. 6 for a similar realization of the controlled-NOT gate)

$$\begin{aligned} U_{\rm CNOT} = {} & \exp(-i\pi/4)U_{2y}(\pi/2)U_{1z}(-\pi/2)U_{2z}(-\pi/2) \\ & \cdot U_{\rm ps}(\pi/2)U_{2y}(-\pi/2) \end{aligned} \quad (5)$$

where the single qubit operations $U_{i\mu}(\theta)$ rotate the qubit i by an angle θ around the axis μ ($u_\mu(\theta) = \exp(-i\sigma_\mu\theta/2)$ acting on i) while leaving the other qubit unchanged.

The switches are important elements in our design, and a valid suggestion for their implementation is the single electron transistor[17]. Here we propose a quiet switch design optimally adapted to our SDS′ qubits. The basic idea derives from frustrating the junctions in a SQUID loop, resulting in a 'phase blockade': combining an SDS′ junction with energy E_d, a π-junction with $E_\pi \ll E_d$, and an s-wave junction with $E_s = E_\pi$ into a (small-inductance) SQUID loop (Fig. 2d), we obtain the following switching behaviour. The phase $\phi = 0$ on the SDS′ junction frustrates the remaining junctions, the loop's energy–phase relation is a constant, $E_{\rm sw}(\phi_\pi = \phi_s - \pi) \equiv 0$, and the switch is open. A voltage pulse coming down the signal lines and switching the SDS′ junction into the $|\pi\rangle$ state changes the phase relation between

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the π- and the s-wave junctions and closes the switch: the energy $E_{sw}(\phi_\pi = \phi_s) = 2E_\pi(1 - \cos\phi_\pi)$ produces the current–phase relation $I = (2e/\hbar)\partial_{\phi_\pi} E_{sw}$, thus suppressing the fluctuations of the phase across the switch. The appropriate voltage pulses could be generated by driving an external SDS′ junction unstable.

The quiet-device concept proposed above relies heavily on the double periodicity of the SD junction. As the second harmonic is strongly suppressed in a SID (s-wave–insulator–d-wave) tunnel junction, a more feasible suggestion for the realization of a $\cos 2\phi$ junction is the SND 'sandwich', where the superconductors are separated by a thin metallic layer N. For a clean metallic layer, the coupling energies for the nth harmonic are large and of the order of $E_J \approx k_F^2 A\hbar v_F/d$, producing the well known saw-tooth shape in the current–phase relation[18] (here, v_F (k_F) denotes the Fermi velocity (wavenumber) in the N layer while d and A are its width and area). In reality, it seems difficult to deposit a clean metallic film on top of a d-wave superconductor, and we have to account for the reduction in the coupling E_J due to the finite scattering length l in the metal layer. Using quasi-classical techniques to describe a dirty SN_dD junction (s-wave–dirty normal metal–d-wave), we obtain a second-harmonic coupling energy $E_d \approx k_F^2 A(\hbar v_F/d)(l/d)^3 \approx (R_Q/R)(l/d)E_T$, where l denotes the scattering length in the normal metal, $R_Q = \hbar/e^2$ is the quantum resistance, R is the junction resistance, and $E_T \approx (\hbar v_F/d)(l/d)$ is the Thouless energy.

The second important device parameter is the tunnelling gap Δ_d, which depends quite sensitively on the coupling to the environment. The usual reduction in the tunnelling probability by the environment[19] is modified if the system is effectively gapped at low energies[20]. This is the case for our $SN_dDN'_dS'$ junction where the low-energy quasiparticle excitations in the metal are gapped over the Thouless energy E_T (ref. 21). The dynamics of the junction are only affected by the presence of virtual processes involving energies larger than E_T, leading to a renormalized capacitance $C_{ren} \approx \hbar/RE_T$ (compare ref. 20) and resulting in the reduced tunnelling gap $\Delta_d \propto E_d \exp[-\nu(R_Q/R)\sqrt{l/d}]$, with ν of the order of unity. Consistency requires that the tunnelling process is 'massive' and hence slow, $\hbar/\tau < E_T$. With a tunnelling time $\tau \approx S/E_d$ ($S \approx \hbar(R_Q/R)\sqrt{l/d}$ gives tunnelling action) we find that the constraint $\hbar/\tau E_T \approx \sqrt{l/d} < 1$ is satisfied. The condition $\Delta_d \ll E_d$ requires the tunnelling gap Δ_d to be small, but large enough in order to allow for reasonable switching times, requiring $(R_Q/R)\sqrt{l/d}$ to be of the order of 10. With typical device dimensions $d \approx 1{,}000$ Å, $l \approx 10$ Å, and $R/R_Q \approx (d/l)(1/Ak_F^2) \approx 1/100$, this condition can be realized. The operating temperature T is limited by the constraint $S/\hbar > E_d/T$, guaranteeing that our device operates in the quantum regime, and the requirement $T < E_T$, that thermal quasi-particle excitations be absent. The first condition takes the form $T \ll \hbar/\tau \approx \sqrt{l/d}E_T$ and is the more stringent. Using the above parameters and a typical value $v_F \approx 10^8$ cm s^{-1}, we obtain a Thouless energy $E_T \approx 1$ K and hence $T \ll 0.1$ K.

An important topic in quantum computation is decoherence. Within our set-up it is the Thouless gap E_T which inhibits the excitation of quasiparticles. The longest trajectories in the $SN_dDN'_dS'$ junction limiting the size of E_T are those connecting the two s-wave superconductors over a path of length $L_{max} \approx 2d^2/l + d_d$, where the first term stems from the diffusive propagation through the two dirty metal layers, and the second term is due to the ballistic trajectory along the node of the d-wave superconductor (of width d_d). The conditions $\xi_d \ll d_d \ll d^2/l$, with ξ_d the coherence length in the d-wave superconductor, then guarantee that the d-wave layer is thick enough to avoid the quenching through the proximity to the s-wave superconductors, while still being thin enough to leave the Thouless gap unchanged. A further source of decoherence are the switches. Within the set-up sketched in Fig. 2d, the voltage pulse triggering the SDS′ junction in the switch is generated through an external junction driven by a current source. We then have to make sure that while the switching signal reaches the SDS′ junction of the switch loop, the external noise is kept away from the qubit's SDS′ junction. Most dangerous is the low-frequency part of the noise spectrum, as it would induce brownian motion of the relative phase in the wavefunction of the qubit. An appropriate filtering can be achieved through a capacitive decoupling (C_{sw}) of the external driven junction generating the pulses and the SDS′ switch, transparent at the high frequencies of the triggering pulse, but suppressing the low-frequency noise of the current source through a factor $(\omega C_{sw}R_B)^2$, where R_B denotes the resistivity of the external current source. Furthermore, the driven junction loop acts as a shunt, producing an additional suppression factor $(e\omega/I_{sw})^2 R_Q/R_B$. □

Received 14 December 1998; accepted 8 March 1999.

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Acknowledgements. We thank A. Kitaev, D. Loss, A. Millis and B. Spivak for discussions. This work was supported by the Fonds National Suisse.

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Metastable ice VII at low temperature and ambient pressure

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Ice exhibits many solid-state transformations under pressure, and also displays a variety of metastable phases[1]. Most of the high-pressure phases of ice can be recovered at ambient pressure provided that they are first cooled below about 100 K. These ice polymorphs might exist on the surfaces of several satellites of the

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