Quantum computing algorithms are realized through unitary operators that result from the temporal evolution of the quantum system under consideration. Typically, these are achieved with a sequence of universal gates [1] which act analogously to the elementary gates of digital computers. Quantum computers hold the promise of exponential speedup with respect to classical computers owing to the massive parallelism arising from the superposition of quantum bits, qubits; for introduc- tions to quantum computing and quantum information processing, see Ref. [2]. Several physical implementations of quantum computing have been suggested; in particular, quantum computing with Cooper pairs [3].

Superconducting circuits [4] feature controlled fabrication and scalability [5]; their drawback is that the leads inevitably couple the qubit to the environment, thereby introducing decoherence [6]. In a superconductor, the number of the Cooper pairs and the phase of the wave function constitute conjugate variables. The majority of investigations has focused either on the charge regime where the number of Cooper pairs is well defined [7], or on the flux regime where the phase is well defined [8]. Qubits utilizing current-driven large Josephson junctions have been tested experimentally [9]. Decisive experimental progress [10] demonstrated that it is possible to realize $10^4$ elementary quantum gates with Josephson-junction qubits. Here we consider Josephson charge qubits.

In this Letter we propose a method to construct arbitrary two- or three-qubit gates by solving the optimization problem of control parameters for a Josephson charge-qubit register. We show that it is possible to numerically find the required control-parameter sequences even for nontrivial three-qubit gates without employing elementary gates. Recently, it has been suggested [11] how to solve a similar problem in the context of holonomic quantum computation [12], where time does not appear as an explicit parameter. Here, the time evolution arises through the Schrödinger equation.

The motivation underlying the investigation of this approach is the need to overcome effects of decoherence. The implementation of a quantum algorithm which is composed of elementary gates is rarely optimal in execution time since the majority of qubits is most of the time inactive; see Fig. 1. The decomposition into elementary gates works extremely well with classical digital computers. However, in the context of quantum computing the number of consecutive operations is strictly limited by the short time window set by interactions with the environment. It is therefore of prime importance to concentrate on the implementations of quantum algorithms [13–15]. We consider the construction of quantum algorithms out of larger building blocks. Whereas careful design and manufacturing can significantly increase the decoherence time, our scenario can serve to reduce the number of the operations needed.

The Josephson charge qubit utilizes the number degree of freedom of a nanoscale Josephson-junction circuit. The states of the qubit correspond to either zero or one extra Cooper pair residing on the superconducting island, usually denoted by $|0\rangle$ and $|1\rangle$, respectively. The Cooper pairs can tunnel coherently to a superconducting electrode. The charging energy of the qubit can be tuned with the help of an external gate voltage, whereas tunneling between the states is controlled with the help of an external magnetic flux.

The explicit single-qubit Hamiltonian for the qubit $i$ is

$$H_{\text{single}}^{i} = -\frac{1}{2}B^{i}_{x}\sigma_{x} - \frac{1}{2}B^{i}_{y}\sigma_{y},$$

where the standard notation for Pauli matrices has been utilized. Here $B^{i}_{x}$ is a tunable parameter which depends

![FIG. 1.](image)

Instead of implementing the three-qubit quantum Fourier transform with the help of elementary gates, we determine a gate that performs the entire three-qubit operation with a single control loop. Note that idle time is avoided.
on the gate voltage, while $B_i^j$ can be controlled with
the help of a flux through the SQUID. Note that setting
$B_i^j = B_i^j = 0$ results in degeneracy. At the degeneracy
point, there will be no change in the physical state of
the system. In the case of single-qubit gates, it is easy to
see from this model that any rotation in $SU(2)$ can be
performed on the qubits. Note that $U(2)$ is not available
since the Hamiltonian is traceless. In general, we cannot
achieve $U(2)^N$ for $N$ qubits since the Hamiltonian of
the entire quantum register turns out to be traceless.
However, the global phase factor is not physical since it
 corresponds to a redefinition of the zero level of energy.

Qubits can be coupled by connecting them in parallel
to an inductor; see Fig. 2. This scenario has the benefit of
allowing for a longer decoherence time and that of being
tunable. The resulting coupling term in the Hamiltonian
between the qubits $i$ and $j$ is then of the form [4]

$$H_{\text{coupling}} = -CB_i^j B_i^j \sigma_\gamma \otimes \sigma_\gamma, \quad \text{(2)}$$

where $C$ is a positive parameter depending on the capaci-
tances of the qubits and also on the inductance. It follows
from Eqs. (1) and (2) that one can apply nontrivial two-
qubit operations by simultaneously turning on the
SQUIDs of the two qubits, although the $\sigma_\gamma$ term will be
turned on as well. All the other qubits must have their
SQUID turned off. On the other hand, one-qubit $\sigma_\gamma$ operations require that all but one SQUID is turned on.
By turning off a SQUID we mean applying a half flux quantum through it. Note that in the present context it
is actually impossible to perform independent operations
on any two subsets of the quantum register due to the
inductive coupling. Since one must also take into account
the decoherence mechanism, it is not practical to let most
qubits reside at their degeneracy point. The question
arises whether it would rather prove more efficient to
try and find some scheme of finding larger quantum
operations, instead of using elementary gates.

To tackle the challenge posed above, we concentrate on
finding quantum gates numerically. The structure of the
Josephson-qubit Hamiltonian is such that it is not imme-
diately transparent how one would actually construct
even the basic controlled-NOT gate. We accomplish this
by considering loops $\gamma(t)$ in the control-parameter space
spanned by $\{ B_i^j(t) \} \text{ and } \{ B_i^j(t) \}$. Therefore, the function

$$\gamma(t) \text{ is of the vector form}$$

$$\gamma(t) = [B_1^j(t) \cdots B_N^j(t) B_1^j(t) \cdots B_N^j(t)]^T, \quad \text{(3)}$$

where we have assumed a register of $N$ qubits. The tem-
poral evolution induces the unitary operator

$$U = T \exp(-i \int \gamma(t) dt). \quad \text{(4)}$$

where $T$ stands for the time-ordering operator and we
choose $\hbar = 1$. The integration is performed along the
path formed by $\gamma(t)$ where the loop starts at the origin,
and, at the degeneracy point. We will restrict the path to a
special class of loops, which form polygons in the pa-
rameter space. Thus the parameters vary in time at a
piecewise constant speed, and none of the parameters is
turned on or off instantaneously. We further set the time
spent in traversing each edge of the polygon equal to
unity. This limitation could be relaxed, in which case
the length of each edge in time would be an additional
free parameter. We also set $C = 1$ in Eq. (2). This can be
achieved by properly fabricating the inductor, but we have
every reason to believe that the algorithm will work for
other choices of $C$ as well. Hence, in order to evaluate
Eq. (4) one needs only to specify the coordinates of the
vertices of the polygon, which we denote collectively as
$X$. Numerically, it is easy to evaluate the unitary op-
erator in a stable manner by further dividing the loop $\gamma(t)$
to tiny intervals that take the time $\Delta t$ to traverse. If $\gamma_i$
denotes all the values of the parameters in the midpoint of
the $i$th interval, and $m$ is the number of such intervals,
then we find to a good approximation

$$U_{X_i} = \exp(-i H(\gamma_m) \Delta t) \cdots \exp(-i H(\gamma_1) \Delta t). \quad \text{(5)}$$

We now proceed to transform the problem of finding the
desired unitary operator into an optimization task.
Namely, any $U$ can be found as the solution of the problem
of minimizing the error functional

$$f(X) = \| U - U_{X_i} \|_F \quad \text{(6)}$$

over all possible values of $X_i$. Here $\| \cdot \|_F$ is the Frobenius
trace norm defined as $\|A\|_F = \sqrt{\text{Tr}(A^TA)}$. The number
of adjustable vertices of the polygon $\nu$ is kept fixed
from the beginning. One needs to have enough vertices
to parametrize the unitary group $SU(2^N)$. The dimension
of this group is $2^{2N} - 1$ and there are $2N$ parameters
for each vertex. Thus, we must have $2N\nu \geq 2^{2N} - 1$. We use
$\nu = 12$ for the three-qubit gates and $\nu = 4$ for the two-
qubit gates. Within this formulation the method of finding
the desired gates is similar to the recently introduced
method of finding holonomic quantum gates [11]. Thus
we again expect the minimization landscape to be rough
and we apply the robust polytope algorithm [16] for the
minimization.

We concentrate on finding two- and three-qubit gates,
since one-qubit gates can be trivially constructed with the
help of Euler angles. A larger quantum gate could be performed by factoring it into two- and three-qubit operations, and the implementation for these could be found numerically. It seems that quantum operations for four, five, or more qubits could be found with the same method, assuming that sufficient computing resources are available. However, even in the case of three-qubit gates the optimization task becomes challenging and we need to use parallel programming. In the parallel three-qubit program, since the function evaluations of \( f(X_\gamma) \) require a major part of the computation, we distribute the workload such that each processor calculates the contribution of a single edge of the polygon. In addition, one processor handles the minimization routine.

Let us turn to the results. First, we attempt to construct a gate equivalent to the controlled-NOT, namely, 

\[
U = \exp\left(\frac{i \pi}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}\right). 
\]

(7)

The phase factor is needed in order for the gate to belong to SU(4). It is already hard to see from the form of the Hamiltonian how this gate would be carried out in the present setting. Figure 3 illustrates an implementation of this gate that has been obtained by minimizing the error function in Eq. (6); the error is negligible. This example clearly illustrates the potential of our method.

As a second example, we construct the two-qubit quantum Fourier transform (QFT). The QFT (see, e.g., Ref. [2]) is given in the case of two qubits by

\[
F_2 = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix}.
\]

(8)

Furthermore, we need to multiply this by \( \exp(i \frac{\pi}{2}) \) in order to find a gate that belongs to SU(4). Figure 4 shows the resulting loop that has been found with the help of the algorithm. In general, the optimization task for two-qubit gates can be performed quite easily with the help of personal computers. However, finding three-qubit gates is already quite time consuming. It proves worth the extra effort to do this, though.

The three-qubit quantum Fourier transform is [2]

\[
F_3 = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^3 & \omega^5 & \omega^6 & \omega^7 \\ 1 & \omega^2 & \omega^6 & \omega^3 & \omega^7 & \omega^5 \\ 1 & \omega^4 & \omega & \omega^2 & \omega^6 & \omega^3 \\ 1 & \omega^5 & \omega^6 & \omega^3 & \omega & \omega^2 \\ 1 & \omega^7 & \omega^5 & \omega^3 & \omega^5 & \omega \\ 1 & \omega^6 & \omega^2 & \omega^3 & \omega^7 & \omega^5 \\ 1 & \omega^4 & \omega^3 & \omega^7 & \omega & \omega^2 \end{bmatrix},
\]

(9)

where \( \omega = \exp(i \frac{\pi}{2}) \). Since \( \det(F_3) = i \) we must set \( \hat{U} = \exp(-i \frac{\pi}{2} F_3) \) such that \( \hat{U} \in SU(8) \). As an evidence of the success of the three-qubit algorithm, we have in Fig. 5 plotted the implementation of the three-qubit Fourier transform. We conclude from these three examples that it is possible to find far more powerful optimal implementations of multiqubit quantum gates with the help of the minimization scheme [17].

To further assess the strength of the technique, we compare the number of steps that are required to carry out the three-qubit Fourier transform using only two-qubit gates with the number of steps required when using the full three-qubit implementation of Fig. 5. The two-qubit implementation [18] requires effectively four gates;
see Fig. 1. Since these gates would have to be performed sequentially, we would need five polygon edges per two-qubit operation. This results in 20 edges for the whole operation. Using elementary gates would require far more edges. Our optimized three-qubit Fourier transform, though, only requires 13 edges. Since each edge contributes the same amount to the operation time, we conclude that our implementation is improved. What is more, not all multiqubit gates can be decomposed as conveniently as the Fourier transform. For them the gain is higher. Thus, increasing the amount of classical computing resources should yield even better results.

In conclusion, we have described how to efficiently construct two- and three-qubit quantum gates for the Josephson charge qubit using numerical optimization. An immediate strength of the present scenario is that one avoids unnecessary idle time during the logical quantum operations. Since the loops are traversed at a piecewise constant speed, and no fields are instantaneously switched, this method of constructing quantum gates should be viable from the experimental point of view as well. The effect of finite fall and rise times of pulses on the quality of quantum gates has been studied recently [19]. Since we do not use pulses but instead interpolate along linear paths in the parameter space, such errors can be avoided. It seems reasonable to construct large-scale quantum algorithms in multiqubit blocks. This can be accomplished by optimizing the gate realization with the help of classical computers.

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Note added.—After submitting our manuscript, work on a parallel switching method was kindly brought to our attention by Burkard et al. [20].

FIG. 5. Control-parameter sequences as functions of time that yield the three-qubit quantum Fourier transform (modulo a global phase). The relative error is on the order of $10^{-5}$ and 100 discretization points were used.

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[17] We have carried out sensitivity analyses on the CNOT and two-qubit QFT gate realizations; the error was found to scale linearly with the rms of the Gaussian noise added at each vertex: error $\propto 6 \times \langle \text{noise} \rangle_{\text{rms}}$.
[18] We assume that one-qubit operations are embedded into two-qubit gates.