Quantum computing with a single molecular ensemble and a Cooper-pair box

Karl Tordrup and Klaus Mølmer
Lundbeck Foundation Theoretical Center for Quantum System Research, Department of Physics and Astronomy,
University of Aarhus, DK-8000 Aarhus C, Denmark

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We propose to encode quantum information in rotational excitations in a molecular ensemble. Using a stripline cavity field for quantum-state transfer between the molecular ensemble and a Cooper-pair-box two-level system, our proposal offers a linear scaling of the number of qubits in our register with the number of rotationally excited states available in the molecules.

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One obstacle which transcends all implementations of a quantum computer [1–4] concerns the extension of current proof-of-principle operations beyond a handful of qubits. At the heart of this obstacle lies the exponential scaling of the Hilbert space dimension with the number of qubits. If one chooses to work with qubits encoded in separate particles, the available state space is exponentially large in particle number, but selective access to individual particles and precise control of the interactions among individual quantum particles presents a formidable challenge. This has spurred interest in quantum systems that intrinsically support a vast Hilbert space. Obvious candidates are molecular quantum systems which easily provide 100 accessible internal rotational and vibrational levels [5,6]. The quantum information capacity of such systems corresponds, however, to a mere $\log_2(100) \approx 6$ qubits, and most molecular implementations to date have not exploited the rich internal structure, but have focused on other advantages provided by molecular systems such as the large intermolecular dipole-dipole coupling [7], switchable interactions [8], and long coherence times [6]. These advantages also make molecules very attractive for hybrid quantum computing schemes involving solid-state, optical, and molecular quantum degrees of freedom simultaneously. Notably, in [9], it has been proposed to trap a mesoscopic molecular ensemble at an antinode of the quantized field of a stripline cavity with a Cooper-pair box (CPB) placed at the adjacent antinode. This setup is illustrated in Fig. 1(a). The energy scale for the stripline cavity mode matches typical energies for rotational excitations of polar molecules, providing a natural interface between the cavity and molecular degrees of freedom. The large electric-dipole moment of polar molecules makes the strong-coupling regime relatively easy to achieve while strong coupling of the field to the CPB has been demonstrated experimentally in [10,11]. Furthermore, by using an ensemble of N molecules one achieves a $\sqrt{N}$ enhancement of the coupling to the weak quantum field compared to the single-molecule vacuum Rabi frequency g. In [9], the essential idea is to counteract the rapid decoherence in a Cooper-pair box by transferring the quantum state to the molecular ensemble for storage of the qubit in a collective molecular excitation between quantum gates.

In this paper we shall present a method for many-qubit quantum computing with a single molecular ensemble and a Cooper-pair box. We shall apply an ensemble of N cold polar molecules with a ground state and K accessible excited states as illustrated in Fig. 1(b). The potentially available Hilbert space for the molecular system is of dimension $(K+1)^N$, but by limiting ourselves to symmetric states with at most one molecule populating each of the excited states, this is reduced to 2^K, the Hilbert space dimension of a K-qubit register.

We assume all molecules are initially prepared in the ground state $|0\rangle$, which is coupled to the excited states $|i\rangle$ through a Raman process involving the cavity field coupling constant g and a classical field $\Omega_i(t)$. Since both fields couple symmetrically to all molecules in the ensemble, elementary excitations produce the symmetric (Dicke) states $|i\rangle = (1/\sqrt{N})\Sigma_j|0_1 0_2 \cdots i_j \cdots 0_N\rangle$ and so forth, where the index j runs over all molecules in the cloud. We define the collective raising operator $m_i^\dagger = (1/\sqrt{N})\Sigma_j|i\rangle_{jj}\langle 0|$. In the regime with only few excited molecules, the collective operators approximately obey the bosonic commutator relation $[m_i, m_i^\dagger] \approx 1$ and the cloud can be treated as a collection of K uncoupled harmonic oscillators.

The conventional approach to encoding qubits in atoms

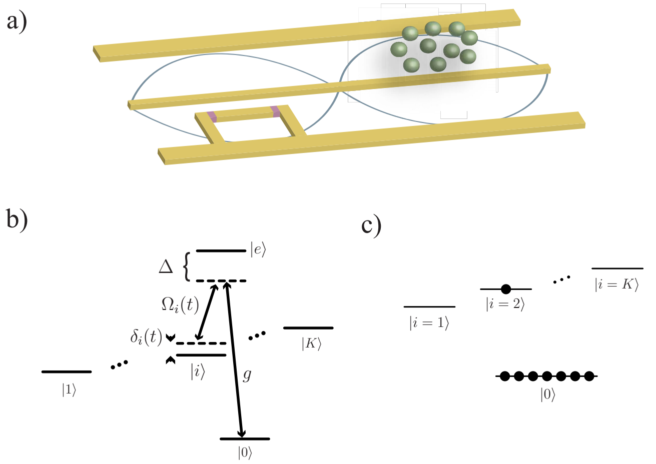

FIG. 1. (Color online) (a) A Cooper-pair box is strongly coupled to a stripline cavity as realized in [10]. Additionally a cloud of cold polar molecules interacts with the quantized cavity field. (b) Internal level scheme for a single molecule. The reservoir state $|0\rangle$ is selectively coupled to each of the excited states $|i\rangle$ by Raman transitions. (c) Encoding of K qubits in the symmetric states of an ensemble of $N > K$ identical particles.

and molecules is to encode a single qubit in a single particle [7,12], or in a single collective degree of freedom in an atomic or molecular cloud [9,13]. However, as was recently proposed in [14], one can encode K qubits in a single cloud of identical particles, each with $K+1$ accessible internal levels by associating the logical register state $|a_1a_2\cdots a_K\rangle$ ($a_i=0,1$) with the collective state $\Pi_i(m_i^\dagger)^{a_i}|0_10_2\ldots0_N\rangle$ with a_i particles populating the ith level, illustrated in Fig. 1(c). The permutation symmetry among particles is important, and, for instance, the logical two-qubit state $|01\rangle$ is an entangled state with no particles populating the excited state $|i=1\rangle$ and a unit population of state $|i=2\rangle$ evenly distributed over all the molecules in the ensemble, in contrast to the conventional simple product-state encoding of the same state. The advantage of this encoding is that it circumvents the need for addressing of individual particles, since qubit access is granted by selective coupling of the ground state to one of the K excited states. The complication of the method lies in the restriction of the dynamics to the specified state space with at most one particle populating each of the excited states and in the operations on these states that depend on the population of the other excited states. In [14] it was proposed to use the Rydberg blockade mechanism for controlled dynamics of neutral atomic ensembles. In this Rapid Communication we shall describe how the cavity field and the two-level system offered by the Cooper-pair box can be used to achieve the same goal for polar molecules.

We now turn to the setup indicated in Fig. 1(a). The Cooper-pair box is a superconducting circuit with an island onto which charge may tunnel through an insulating barrier as described by a phenomenological Hamiltonian, $H=-(E_J/2)\Sigma_n|n\rangle\langle n+1|+|n+1\rangle\langle n|$ [15]. Due to the quadratic nature of the electrostatic interaction, the energy levels are nonequidistant, and using resonant transitions only, the system may at cryogenic temperatures be restricted to the two lowest quantum states with corresponding raising and lowering operators σ^+ and σ^-. The CPB is mounted on a superconducting stripline cavity which can hold a cavity field with creation and annihilation operators $c^\dagger$ and c with very modest field damping [16]. The combined system CPB-cavity system is governed by the Jaynes-Cummings-type Hamiltonian

$$H_{\mathrm{CPB}} = g_c(\sigma^- c^\dagger + \sigma^+ c) + \delta_{\mathrm{CPB}}(t)\sigma^+\sigma^-, \qquad (1)$$

where $\delta_{\mathrm{CPB}}(t)=\omega_{\mathrm{CPB}}(t)-\omega_c$ is the tunable CPB detuning with respect to the cavity field. A number of phenomena related to the Jaynes-Cummings Hamiltonian in quantum optics have been observed in the CPB-cavity system [10,11], and two-qubit gates on two Cooper-pair boxes coupled to a single-cavity field mode have recently been demonstrated [4]. The molecular ensemble is addressed by a Raman transition involving the cavity field and a classical field with tunable frequency and real amplitude $\Omega_i(t)$ [see Fig. 1(b)]. In the rotating-wave approximation after adiabatic elimination of the excited state $|e\rangle$ the coupling of the cavity field to the ith molecular qubit is described by

$$H_{\mathrm{M}} = g_i(t)(m_i c^\dagger + m_i^\dagger c) + \delta_i(t) m_i^\dagger m_i. \qquad (2)$$

Here $g_i(t)=\Omega_i(t)g\sqrt{N_0}/2\Delta$ is the effective coupling strength with Δ the detuning with respect to the intermediate excited state and $\delta_i(t)$ is the two-photon Raman detuning of level $|i\rangle$; cf. Fig. 1(b). Coupling by higher-order Raman processes with the cavity field and multiple classical field components allows exploration of a wider range of molecular states for which Eq. (2) applies with modified expressions for $g_i(t)$.

We will now describe how quantum information can be encoded and processed in the combined system. Initially the molecular ensemble is prepared with all molecules in the zero state corresponding to all qubits set to the value 0. We now need to specify how to carry out reliable one- and two-bit gates on the system, and specifically for the ensemble encoding, we have to ascertain that no register state is populated by more than a single molecule. The cavity and CPB are also prepared in their ground states, and SWAP operations of arbitrary unknown states between any qubit component of the molecular memory and the CPB via the cavity field, combined with an arbitrary single qubit rotation of the CPB two-level system by resonant driving with a classical field, implements this rotation on the desired single qubit of the register. As a fully entangling two-qubit gate we propose to SWAP one molecular ensemble qubit to the CPB and then SWAP another molecular ensemble qubit to the cavity field. The CPB-cavity interaction can then provide a state-dependent phase remaining with the two-qubit states when they are finally returned to the collective molecular ensemble states. Before presenting the details of these processes we note that the main elements of these steps are, indeed, very similar to the ideas for quantum computing with atoms coupled via a cavity field [17] and with trapped ions coupled to each other via their collective motional degree of freedom [18]. But we emphasize the significant difference that our molecules do not need to be individually addressed and that we need to pass the cavity excitation through the Cooper-pair box to restrict the Hilbert space to two states per qubit degree of freedom and to provide the interaction in the system.

The SWAP operations can be realized by adiabatically sweeping the detunings across resonance. When transferring a molecular state to the empty cavity the coupling $g_i(t)$ is turned on with $\delta_i(t=0)/g_i \gg 1$. As $\delta_i(t)$ passes through resonance each basis state adiabatically evolves into the corresponding dressed state:

$$|+,n\rangle = \cos(\theta)|1\rangle_m|n\rangle_c + \sin(\theta)|0\rangle_m|n+1\rangle_c, \qquad (3)$$

$$|-,n\rangle = -\sin(\theta)|1\rangle_m|n\rangle_c + \cos(\theta)|0\rangle_m|n+1\rangle_c, \qquad (4)$$

with $\tan(2\theta)=2g_i\sqrt{n+1}/\delta_i(t)$ and energies $E_{\pm,n}=\frac{1}{2}\delta_i(t)\pm\frac{1}{2}\sqrt{\delta_i^2(t)+4g_i^2(n+1)}$. Here $n+1$ is the number of elementary excitations—i.e., $n=0$ for the states $|0\rangle_m|1\rangle_c$ and $|1\rangle_m|0\rangle_c$ and $n=1$ for $|1\rangle_m|1\rangle_c$. As a result each state acquires a nonlinear phase relative to the ground state of $\varphi_{\pm,n}=\frac{1}{2}\int_0^T-\delta_i(t)\mp\sqrt{\delta_i^2(t)+4g_i^2(n+1)}dt$. Thus the logical state $|1\rangle$ acquires a phase relative to $|0\rangle$ while following $|+,0\rangle$ (see Fig. 2, left panel). When returning the state to the ensemble the $|1\rangle$ component can either be made to follow $|+,0\rangle$ (by sweeping from negative to positive detuning) or $|-,0\rangle$ (by sweeping from positive to negative detuning). By choosing the latter option the total dynamical phase $\exp\{-i\int_0^T[E_+(t)+E_-(t)]dt\}$ is exactly canceled for any sweep

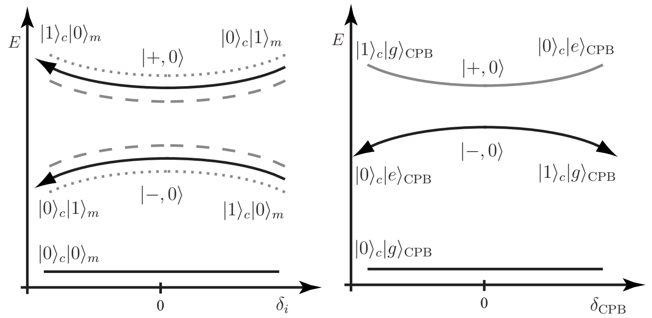

FIG. 2. Left: in order to transfer a molecular state to the cavity we turn on a far-detuned field with $\delta_i/g_i \gg 1$ and sweep through resonance adiabatically following the dressed state $|+,0\rangle$. To transfer the state back to the molecular ensemble the field is again turned on at $\delta_i/g_i \gg 1$, this time following the $|-,0\rangle$ state through resonance. Phase errors due to fluctuating N_0 (illustrated by the dashed and dotted lines) are exactly canceled, leaving only a geometric phase of $e^{-i\pi}$. Right: when transferring states between the cavity and CPB one must follow the same path back and forth. Hence the geometric phase vanishes. Since there is no fluctuation in the interaction strength g_c, the dynamical phase can be tailored to 0 mod 2π.

that is antisymmetric about $t=T/2$. The $|1\rangle$ state then only acquires a geometric phase of $e^{-i\pi}$. The effective coupling of the ground to any particular excited states is amplified by the number of participating molecules; i.e., it is $g\sqrt{N_0}$ with N_0 the number of ground-state molecules. This number has a quantum mechanical uncertainty when some of the other excited states are in superposition states of being populated and unpopulated. The relative variation in the coupling strength due to this uncertainty can be suppressed by requiring $N \gg K$, but we observe that since we accumulate opposite phases in the two adiabatically swept passages, indicated by the dotted($N>N_0$) and dashed ($N<N_0$) curves in the figure, the difference will effectively cancel.

The phase dynamics is most easily visualized by viewing the dynamics as a spin-1/2 precessing about a fictitious magnetic field $\boldsymbol{B}(t)=-(g_i,0,\frac{1}{2}\delta_i(t))$. Two consecutive sweeps of $\delta_i(t)$ in the same direction correspond to a 2π rotation of $\boldsymbol{B}(t)$, giving a geometric phase of $e^{-i\pi}$. This SWAP operation thus incurs an extra single-qubit Z gate which must be absorbed into future operations. When transferring between the cavity and CPB we have an *always on* interaction g_c and two consecutive sweeps must be in opposite directions (see Fig. 2, right panel). This corresponds to following the $|+,0\rangle$ ($|-,0\rangle$) state twice, and hence there is no cancellation of the dynamical phase. However, in this case the geometric phase vanishes since the fictitious **B** field traces out a path enclosing a vanishing solid angle. The sweep may then be chosen such that the dynamical phase becomes 0 mod 2π since there is no fluctuation in the coupling g_c. For instance, the cubic parametrization $\delta_{\rm CPB}(t)=\delta_0(2t/T-1)^3$ with $\delta_0 = 19.24 g_c$ and $T=20.77 g_c^{-1}$ gives a cancellation of the dynamical phase. The cubic form was chosen since it is odd about $t=T/2$ and offers faster implementation than a linear chirp while remaining in the adiabatic limit.

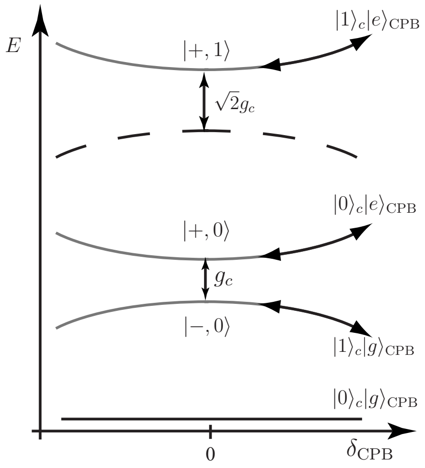

FIG. 3. A conditional phase shift is performed by exploiting that the dressed-state energies are nonlinear in the excitation number n. Starting at $\delta_{\rm CPB}(0)/g_c \gg 1$ the CPB is tuned close to resonance $[\delta_{\rm CPB}(T/2) \sim g_c]$ and back to end at $\delta_{\rm CPB}(T)/g_c \gg 1$. The functional form of $\delta_{\rm CPB}(t)$ is chosen such that $\varphi_{+,1}=\pi$ mod 2π while $\varphi_{\pm,0}=0$ mod 2π. The dashed line represents the dressed state $|-,1\rangle$ which at $\delta_{\rm CPB}/g_c \gg 1$ corresponds to $|2\rangle_c|g\rangle_{\rm CPB}$—i.e., a doubly excited state which is not part of the computational Hilbert space.

To implement a single-qubit gate on qubit i we transfer the molecular state to the cavity by tuning $\delta_i(t)$ across resonance and then transfer the state to the CPB by a similar sweep of $\delta_{\rm CPB}(t)$. A single-qubit gate may then be implemented on the CPB using microwave pulses [19] whereafter the state is transferred back to the ensemble via the cavity. To implement two-qubit entangling operations we make use of the cavity-CPB coupling described by Eq. (1). The control qubit is transferred to the CPB and the target qubit is subsequently transferred to the cavity field as described above. From an initial detuning of $\delta_{\rm CPB}/g_c \gg 1$ the CPB detuning is tuned close to resonance and back, the computational states evolving adiabatically along the dressed states as seen in Fig. 3. In order to implement a fully entangling controlled phase operation the functional form of $\delta_{\rm CPB}(t)$ must be chosen such that $\varphi_{\pm,0}=0$ mod 2π and $\varphi_{+,1}=\pi$ mod 2π. We find that parametrizing $\delta_{\rm CPB}(t)=a(2t/T-1)^2+b$ with $a=33.05 g_c$, $b=0.6664 g_c$, and $T=58.07/g_c$ produces a controlled phase gate with near unit fidelity.

Let us now address the feasibility of our proposal with current physical parameters. For the Cooper-pair box, the dominant source of decoherence is second-order charge noise, which is minimized by operation at the so-called sweet spot, leading to dephasing times of the order $T_2 \sim 1\ \mu$s [20]. By comparison the vacuum Rabi frequency of the CPB-cavity field coupling is of the order $g_c \sim 2\pi \times 50$ MHz, so for single-qubit rotations on the CPB we obtain $g_c T_2 \sim 300$; i.e., one can implement on the order of 300 CPB-cavity SWAP operations before the qubit decoheres. The conditional phase gate we have proposed has a gate time of $T=58.07 g_c^{-1}$ giving $T/T_2 \sim 0.1$. This ratio can be improved by more than an order of magnitude by replacing the conventional CPB with a recently improved so-called transmon design [20], which operates in a regime where the dominant decoherence process is relaxation with $T_1 \sim 16\ \mu$s. The coherence time of the molecular ensemble is limited mainly by the collision rate and by coupling due to the long-range dipole-dipole interaction. In a magnetic trap, at $T=1$ mK the scattering rate due to the asymptotic r^{-6} interaction is estimated to be $\gamma \lesssim 2\pi \times 700$ Hz [9]. In an electrostatictrap the induced dipole moment μ_{ind} leads to an r^{-3} interaction, but at $T=1$ mK and $\mu_{\text{ind}} < 1$ D, the above estimate for the scattering rate still holds and we conclude that the interactions within the molecular ensemble should not significantly lower the effective decoherence time. With photon loss rates down to $2\pi \times 10$ kHz and realistic values of g_i up to $2\pi \times 10$ MHz [9], with current technology one could implement hundreds of gates, sufficient to provide proof of concept for the present scheme and to carry out simple error correction algorithms.

In conclusion we have described a system which with current technology could provide quantum computation with an appreciable number of qubits. The ensemble encoding we have used is applicable to systems which contain a saturable element such as the Cooper-pair box which furthermore serves to provide an entangling conditional phase gate. The molecular ensemble provides an efficient encoding scheme for many easily accessible qubits and long coherence times which may be improved even further by adopting a crystalline ensemble in which collisions are suppressed. If additionally one chooses a trapping scheme which is independent of the rotational state, there exist certain "magic" configurations for which detrimental coupling to the phonon spectrum is completely suppressed [21]. Potentially in future applications several ensembles could be coupled to an array of Cooper-pair boxes in several interconnected cavities, providing scalability as well as the benefit of parallel processing. Further improvements in the present work could include the application of optimal control theory [6] to improve the gate time for the conditional phase shift as well for the SWAP operations.

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