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Abstract. We describe the integration of polar molecules with mesoscopic solid state devices in a way that produces robust, coherent, quantum-level control with applications for quantum information processing. The exceptional features of polar molecules, i.e. long-lived rotational states in combination with electric dipole moments of several Debye, provide the necessary ingredients to achieve strong coupling to the quantized field of a high-Q microwave cavity. We discuss two scenarios, where quantum information is stored either in rotational states of a single molecule or in collective spin excitation of an ensemble of molecules. In the latter case we benefit from an enhanced coupling strength, which allows a coherent transfer of quantum information between molecules and solid state qubits.

Keywords: polar molecules, microwave resonators, quantum information processing
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INTRODUCTION

The recent development of new cooling and trapping technologies for the production of cold and ultra-cold molecules [1] opens new perspectives for the manipulations of molecules on a quantum level in a way that currently is only achieved for atomic systems [2, 3, 4]. In contrast to atoms or ions, the rotational degrees of freedom of molecules in combination with electric dipole moments provide additional features which might be exploited for trapping and quantum information processing [5, 6, 7] with static and microwave electric fields. Due to the large dipole moments of $\mu \sim 5$ Debye, polar molecules interact strongly with electric fields, which is a key property for coherent interactions solid state devices such as superconducting microwave cavities [8] or charge qubits [9, 10].

Here we show that trapping the molecules at short distances from a superconducting transmission line resonator leads to a coherent coupling of the molecular rotational states with the quantized microwave field of the resonator. This coupling can be used to build a scalable quantum processor where qubits are stored in rotational states of polar molecules and the transmission line cavity serves as a coherent quantum bus for two qubit gate operations as well as cooling, and high fidelity readout [11]. By adopting molecular ensembles instead of a single molecules, we benefit from an additional col-

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lective enhancement of the molecule-cavity coupling, which allows a coherent exchange of quantum information between molecules and solid state qubits, e.g. in the form of a Cooper pair box (CPB) coupled to the same cavity [8]. In such a hybrid device [12] molecular ensembles find applications as long-term quantum memories and optical interconnects for solid state qubits .

LONG-LIVED MOLECULAR QUBIT STATES

The level structure of diatomic molecules [13] in the electronic and vibrational ground state is dominated by the rigid rotor Hamiltonian $H_{\rm rot} = B\mathbf{N}^2$, where $\mathbf{N}$ is the rotational angular momentum and $B \sim 2\pi \times 10$ GHz is the rotational constant. This Hamiltonian gives energy levels $E_N = BN(N+1)$ that are $(2N+1)$-fold degenerate, corresponding to the different projections m_N, as shown in Fig. 1 a). Due to a negligible radiative decay of rotational states and the anharmonicity of the rotor spectrum two states with quantum numbers N and $N+1$ represent a long-lived qubit which can be selectively coupled by electric microwave fields of frequency $\omega \approx \omega_{01} = 2B(N+1)/\hbar$. For example, we can choose the two states $|0_r\rangle = |N=1, m_N=0\rangle$ and $|1_r\rangle = |N=2, m_N=0\rangle$ as a (rotational) single molecule qubit. These two states are 'low-field-seekers' meaning that both qubit states can be trapped simultaneously using electrostatic potentials.

As we discuss below, rotational levels are sensitive to electric field fluctuations and, in the case of molecular ensembles, affected by inelastic collisions. To improve the lifetime of molecular qubits it is favorable to encode quantum information in Zeeman or hyperfine sublevels within the same rotational manifold. For example, in the case of CaF the spin of the unpaired electron, $\mathbf{S}$, couples to the molecule rotation according to $H_{SR} = \gamma_{sr}\mathbf{SN}$ with $\gamma_{sr} \sim 2\pi \times 100$ MHz. The coupling results in a spin rotation splitting (ρ-doubling) for rotationally excited states. In addition, there are hyperfine interactions with a nuclear spin $I = 1/2$ which in particular lead to a splitting of the ground state $N = 0$, into $F = 0$ and 1 states, with $\mathbf{F} = \mathbf{N} + \mathbf{S} + \mathbf{I}$ the total angular momentum. Fig. 1 shows the resulting hyperfine manifolds for the two lowest rotational states $N = 0, 1$ for the example of CaF. For storage, quantum information may be encoded in robust hyperfine qubits, for example in the 'clock states' $|0_h\rangle = |F=0, m_F=0\rangle$ and $|1_h\rangle = |F=1, m_F=0\rangle$ of the rotational ground state. In that case the qubit states are highly protected from electric and magnetic field fluctuations while they can still be coupled via a two photon Raman process involving two microwave fields of appropriate polarization and frequency as indicated in Fig.1 c). Trapping of rotational ground state molecules can be achieved using electric rf- or microwave potentials [14, 15].

A SCALABLE MOLECULAR QUANTUM PROCESSOR

Cavity QED with polar molecules. Superconducting coplanar stripline resonators [11] of length L and electrode spacing d can be used to confine microwave fields to an extremely small volume [16], $V \sim d \times d \times \lambda \ll \lambda^3$, where $\lambda \approx L \approx 1$ cm is the resonant wavelength. One important consequence is the large vacuum Rabi frequency $g = \wp\mathscr{E}_0/\hbar$ for molecules located close to such a resonator, enabling coherent coupling

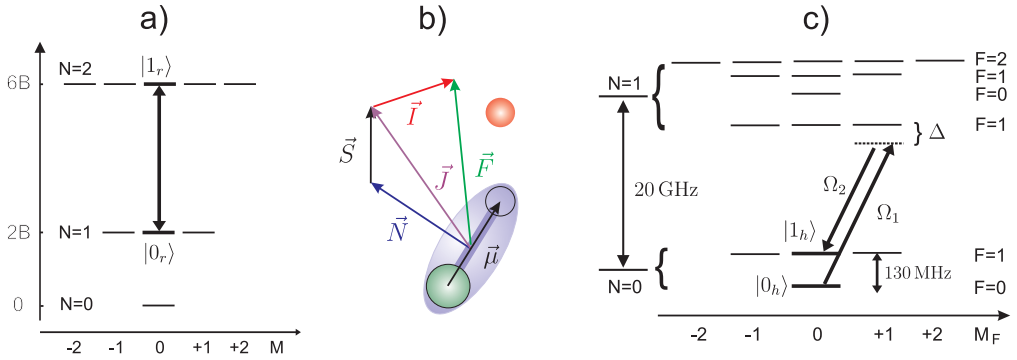

FIGURE 1. a) Spectrum of a rigid rotor, $H = B\mathbf{N}^2$. b) Coupling of angular momentum vectors: The spin-rotation interaction couples the rotation of the nuclei (**N**) with the spin of the electron (**S**) to a combined angular momentum $\mathbf{J} = \mathbf{N} + \mathbf{S}$. Hyperfine interactions couple **J** and the nuclear spin **I** to the total angular momentum vector $\mathbf{F} = \mathbf{J} + \mathbf{I}$. c) Hyperfine manifolds of the lowest two rotational states for the example of CaF. The spectrum is calculated from the Hamiltonian $H_M = B\mathbf{N}^2 + \gamma_{sr}\mathbf{N}\cdot\mathbf{S} + b\mathbf{S}\cdot\mathbf{I} + c(\mathbf{n}\cdot\mathbf{S})(\mathbf{n}\cdot\mathbf{I})$, with $B = 2\pi \times 10.15$ GHz, $\gamma_{sr} = 2\pi \times 39.7$ MHz, $b = 2\pi \times 109$ MHz, and $c = 2\pi \times 41.2$ MHz. Hyperfine qubits $|0_h\rangle$ and $|1_h\rangle$ are coupled via two a two photon Raman process with corresponding Rabi frequencies Ω_i and detuning Δ. For a molecule-cavity coupling one of the classical microwave fields is replaced by the quantized field of the cavity, e.g. $\Omega_1 \rightarrow g$.

of the molecule to the quantum state of the resonator field. Here $\wp$ is the transition dipole matrix element and $\mathscr{E}_0 \propto V^{-1/2}$ is the zero-point electric field; $\wp \approx 0.5\mu$ under the relevant conditions.

When the microwave field is confined to a resonator and is quantized, the coupling becomes the well-known [17] Jaynes-Cummings Hamiltonian $\hat{H} = -\hbar g(\hat{a}^\dagger\hat{\sigma}^- + \hat{a}\hat{\sigma}^+)$, where $\hat{a}$ is the annihilation operator for the resonator mode, $\hat{\sigma}^- = |0_r\rangle\langle 1_r|$ is the lowering operator for the molecule, and $|0_r\rangle, |1_r\rangle$ are the two qubit states coupled by the field. For a molecule trapped at a height $z \lesssim d$ above the stripline the value of g is given by (see also [18])

$$g \approx \frac{\wp}{\hbar}\sqrt{\frac{\hbar\omega_c}{2\pi\varepsilon_0 d^2 L}} \approx 2\pi \times 50\,\mathrm{kHz} \times \frac{1}{d[\mu\mathrm{m}]}\,. \tag{1}$$

With the help of electrostatic potentials, for example using the idea of an electric Z-trap as proposed in Ref. [11], polar molecules can be strongly confined at distances $z \approx 0.1 - 1\,\mu$m above the resonator, with resulting coupling constants of $g/2\pi \approx 50 - 500$ kHz. Since high Q resonators of internal Q's of 10^6 have been demonstrated [19, 8], the strong coupling regime of cavity QED [20, 21] , $g > \kappa$, can be reached and a coherent quantum state exchange between the polar molecule and the resonator field is possible.

The discussion so far has ignored dephasing of superpositions of rotational qubit states due to the ubiquitous 1/f noise in the electrodes and thermal motion in the trap. Decoherence due to voltage noise is determined by the electric field sensitivity of the rotational splitting, $\partial\omega_{01}/\partial\mathscr{E}$, and is minimized for a specific offset field value, $\mathscr{E}_{DC}^{\mathrm{sweet}} \approx 3B/\mu$, – a "sweet spot" – for which the level splitting $\omega_{01} = (E_1 - E_0)/\hbar$ is to first order independent of the electric field $\mathscr{E}$. The analysis of the residual dephasing of rotational qubits given in Ref. [11] predicts Gaussian decay of qubit superpositions with a characteristic rate $\gamma^* \approx \bar{n}^2 \times 1\,$kHz, with $\bar{n}$ the thermal occupation number in the trap.

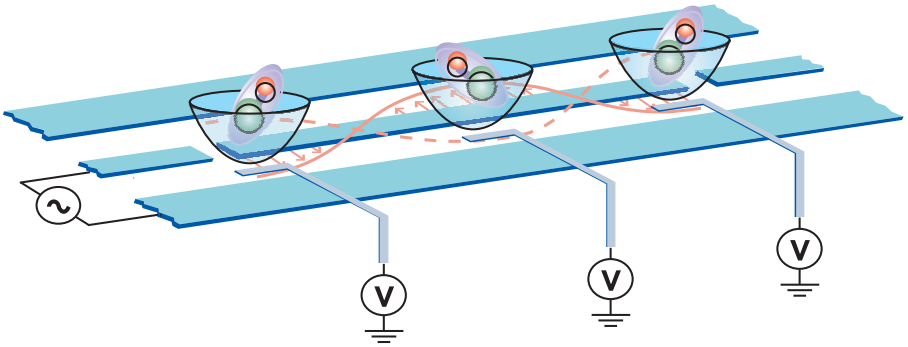

FIGURE 2. A scalable all-electrical implementation of a quantum computer with polar molecules and microwave resonators. Quantum information is encoded in rotational or hyperfine states of polar molecules which are electrically trapped close to the surface of a superconducting stripline cavity. Long-range coherent two qubit operations are mediated by the quantized field of the microwave resonator.

Thus, cooling of the molecular motion is crucial for long-lived rotational coherences. This problem can be solved using cavity assisted sideband cooling, where the damping of the microwave cavity provides the dissipation channel [11].

Long-range quantum coupling of molecular qubits. We now consider coherent interactions of polar molecules through the capacitive, electrodynamic coupling to superconducting transmission line resonators [16, 18]. For simplicity, we consider a $\sqrt{\text{SWAP}}$ operation between a pair of rotational qubits. We use an off-resonant interaction with detuning Δ between resonator and qubit, with the molecules located at voltage nodes along the resonator. Assuming $\Delta \gg g$ and adiabatically eliminating the resonator degree of freedom, we find an interaction of the form

$$H_{int} = \hbar \frac{g^2}{\Delta} \left(\hat{\sigma}_1^+ \hat{\sigma}_2^- + \hat{\sigma}_1^- \hat{\sigma}_2^+ \right), \tag{2}$$

where g^2/Δ is the interaction rate and $\hat{\sigma}_i^- = |0_r\rangle\langle 1_r|_i$ is the lowering operator for ith molecule. This effective exchange interaction can be used to map coherent superpositions from one quantum bit to another in time $\tau = \pi\Delta/2g^2$, thus enabling a universal two-qubit gate [22]. Note that at large molecule-resonator detuning ($\Delta \gg \kappa$), the resonator mode is only virtually occupied, so that cavity decay has little effect: the probability of error due to spontaneous emission of a photon during the two-bit gate is $p_{sp} = \kappa g^2/\Delta^2\tau = (\pi/2)(\kappa/\Delta)$. While slower gate speed (at large detuning Δ) results in reduced p_{sp}, it also results in increased probability of dephasing $p_{dep} = (\gamma^*\tau)^2$. The overall probability of error $p_{err} = p_{sp} + p_{dep}$ is minimized by choosing $\Delta^* = \sqrt[3]{g^4\kappa/\pi\gamma^{*2}}$, resulting in a total error probability $p_{err} \approx \left(\kappa\gamma^*/g^2\right)^{2/3}$. For example, with $\kappa = 2\pi \times 10$ kHz ($Q = 10^6$), $g = 2\pi \times 200$ kHz, and $\gamma^* \sim 2\pi \times 1$ kHz we find that at the optimal detuning a probability of error is well below one percent. Thus, high-fidelity two-qubit operations between remote qubits are possible.

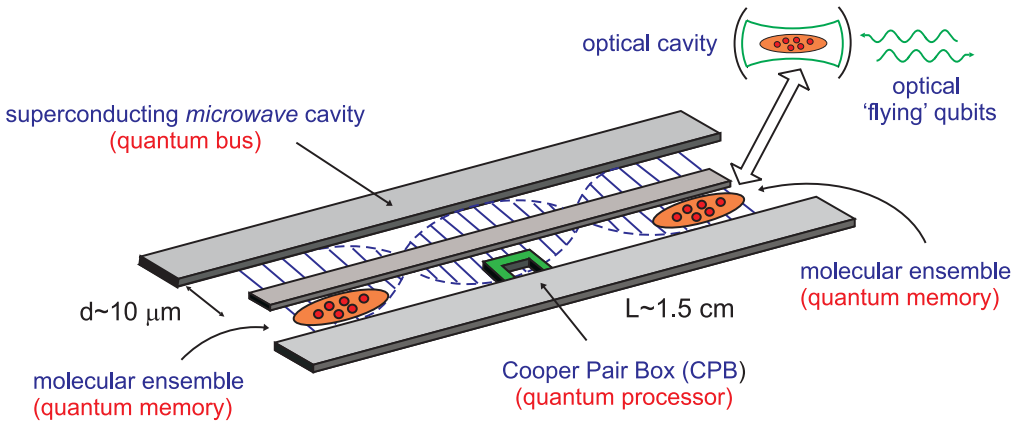

FIGURE 3. Schematic setup of a hybrid quantum processor where the Cooper pair box represents the solid state quantum processor and the molecular ensembles serve as long-lived quantum memories. The processor and the memory are connected by a quantum bus, the quantized field of a strip line cavity. Integrated optical cavities provide a coherent interface to flying qubits.

Conclusion. In combination with on-chip trapping techniques as well as cavity assisted cooling and state detection [16, 11], the high fidelity gate operation between polar molecules provide the basic ingredients for the implementation of a quantum computer, which is within experimental reach (see Fig. 2). Note that in contrast to proposals for scalable quantum computers with trapped ions [23], the scalability in the present architecture is achieved by long-range interactions mediated by the stripline cavity, combined with the advantages of all-electrical control via microwave signals on a chip.

ENSEMBLE QUBITS FOR HYBRID QUANTUM PROCESSORS

We have shown that the superconducting stripline cavity provides a coherent quantum bus between two molecular qubits. By replacing one of the molecules with solid state qubit, e.g. a Cooper pair box (CPB), the cavity may also serve as a coherent interface between molecular and solid state qubits. Since solid state qubits decohere much faster, a coherent exchange of quantum information in such a hybrid configuration requires resonant coupling and therefore molecule-cavity coupling constants of $g/2\pi \geq 1$ MHz. This regime can be reached by adopting a molecular ensemble instead of a single polar molecule, where we benefit from the enhancement of the coherent coupling, $g\sqrt{N}$, with N the number of molecules. This strong coupling between the molecular ensembles and the circuit QED system [8] (a CPB coupled to a microwave cavity) also opens the possibility of a solid state based readout of molecular qubits. In addition, qubits stored in the molecular ensemble can be converted to "flying" optical qubits, using techniques demonstrated for atomic ensembles [24, 25, 26, 27, 28]. This provides a natural interface between mesoscopic quantum circuits and optical quantum communication.

In the following we outline the properties of such a hybrid scenario [12] where molecular ensembles and a CPB are coupled to the common mode of a superconducting

cavity (see Fig. 3). The cavity is assumed to be strongly coupled to a CPB representing a circuit QED system, as realized in recent experiments at Yale [8]. As discussed above, molecular spectroscopy allows us to identify long-lived states, for example in the form of a hyperfine qubit $|0\rangle \equiv |0_h\rangle$, $|1\rangle \equiv |1_h\rangle$ in the ground rotational manifold. Starting with a cloud of N molecules prepared in $|0\rangle_m \equiv |0_1 0_2 \ldots 0_N\rangle$ coupling to a microwave or cavity field leads to excitations in the form of symmetric Dicke states, $|1\rangle_m \equiv 1/\sqrt{N}\sum_i |0_1..1_i..0_N\rangle \equiv m^\dagger|0\rangle_m$ *etc.* For weak excitation the operator m obeys approximate harmonic oscillator commutation relations $[m, m^\dagger] \approx 1$, and the ensemble excitations are conveniently described as a set of harmonic oscillator states $|0\rangle_m$, $|1\rangle_m \equiv m^\dagger|0\rangle_m$ *etc.* Here we show that we can use the lowest two of these states as ensemble qubits, which can be manipulated by coupling them to the superconducting cavity and a CPB.

The dynamics of the coupled system (see Fig. 3) can be described in terms of a Hamiltonian $H_{\rm sys} = H_C + H_M + H_{CM}$, which is the sum of a Jaynes-Cummings type Hamiltonian for the circuit QED system H_C, a Hamiltonian for the (spin) excitations of the molecular ensembles H_M, and the coupling of the molecules to the cavity H_{CM}. In a frame rotating with the cavity frequency ω_c, the circuit QED Hamiltonian has the form

$$H_C = -\hbar\delta_c(t)|e\rangle\langle e| + \hbar g_c(|e\rangle\langle g|\hat{a} + |g\rangle\langle e|\hat{a}^\dagger)\,. \tag{3}$$

Here $|g\rangle$ and $|e\rangle$ denote the ground and the first excited eigenstate of the CPB at the charge degeneracy point representing a charge qubit with a (tunable) transition frequency $\omega_{cq}(t)$ and a detuning from the cavity $\delta_c(t) = \omega_c - \omega_{cq}(t)$. The Hamiltonian describing the internal excitations of the molecular ensembles, $i = 1, 2$, and the coupling of ensemble states to the stripline cavity takes the form

$$H_M + H_{CM} = -\hbar\sum_i \delta_{m,i}(t)\, m_i^\dagger m_i + \sum_i \hbar g_{m,i}(t)\,\left(m_i^\dagger \hat{a} + m_i \hat{a}^\dagger\right)\,. \tag{4}$$

The derivation of the Hamiltonian (4) is outline in Ref. [12] where the $g_m^i(t)$ are identified as effective Raman couplings and $\delta_{m,i}(t)$ as individually controllable Raman detunings. We note the basics structure of $H_{\rm sys}$. The ensemble excitations and the cavity represent a system of coupled harmonic oscillators interacting with a two-level system (CPB) with controllable coefficients.

In general, $H_{\rm sys}$ provides the basic ingredients for (i) coherent swap operations between charge, cavity and ensemble qubits, (ii) rotations of a single ensemble qubit via the charge qubit, and (iii) 2-qubit entanglement operations between two ensemble qubits, where the charge qubit plays the role of a nonlinearity. For example, we can prepare the CPB in an arbitrary superposition state $\alpha|g\rangle + \beta|e\rangle$ and by an appropriate control sequence this state can be swapped over to the cavity, and is finally stored in one of the molecular ensembles, and vice versa:

$$(\alpha|g\rangle + \beta|e\rangle)\,|0\rangle_c|0\rangle_m \leftrightarrow |g\rangle\,(\alpha|0\rangle_c + \beta|1\rangle_c)\,|0\rangle_m \leftrightarrow |g\rangle|0\rangle_c\,(\alpha|0\rangle_m + \beta|1\rangle_m)\,. \tag{5}$$

To realize universal two qubit gate operations between two ensemble qubits the state of the ensembles is first mapped onto photon states of the cavity on which the CPB can act as a non-linear phase shifter. The details of such a gate sequence are given in Ref. [12].

The fidelity of these gate operations depends on various sources of decoherence. In the Yale experiment [8], the circuit QED system realizes the strong coupling regime with vacuum Rabi frequency $g_c \approx 2\pi \times 50$ MHz. The decoherence of the charge qubit is dominated by the dephasing rate $T_2^{-1} \approx 2\pi \times 0.5$ MHz, while the photon loss rate is $\kappa/2\pi = 1$ to 0.01 MHz, i.e. the charge qubit is the dominant source of decoherence. For a cloud of $N \approx 10^4$ to 10^6 molecules, trapped at convenient distance $10\,\mu$m above the strip line cavity one can reach the regime of strong cavity - ensemble coupling $g_m/2\pi \approx 1..10$ MHz [12]. The resulting gate error for swap operations or two qubit gates is then the sum of the gate error within the circuit QED system, $p_c \approx (gT_2)^{-1}$, and the transfer error between cavity and ensemble states, $p_m \approx \kappa/g_m$. The parameters stated here show, that a high fidelity transfer of quantum information between hybrid qubits can be achieved.

Ensemble quantum memory. The long coherence time of molecular hyperfine states in combination with a strong (Raman) coupling to microwave cavities qualify molecular ensembles as a good quantum memories for solid state qubits. The lifetime of such an ensemble quantum memory realized by a gas of cold molecules is fundamentally limited by collisional dephasing. Here it is important that collective excitations of the form $|1\rangle_m$ are quite robust against local decoherence effects [29, 12]. Especially for constant density, the collisional decoherence rate does not scale with the number of molecules. Therefore, although the precise molecular scattering are at present unknown, dephasing rates of well below 1 kHz can be expected [12]. Finally, we note that collisional dephasing can be avoided all together, if the ensemble is prepared in a crystalline phase of dipolar gases with dipole moments induced and aligned by a DC electric field under 2D trapping conditions [30].

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