## Erratum: Quantum phase gate and controlled entanglement with polar molecules [Phys. Rev. A 75, 033414 (2007)]

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In our original paper, to derive Eq. (24) the quantum state  $|++\rangle$  was erroneously considered as an eigenstate of the total bimolecular Hamiltonian. As a consequence, the mechanism introduced for the implementation of the conditional  $\pi$  two-qubit phase gate does not perform the desired operation.

We correct this error by introducing an alternate mechanism for the implementation of the desired phase gate. This mechanism is still based on the excitation of both molecules, thus circumventing individual addressability. This alternate scenario is easier to implement than our original proposal since it only involves single photon absorptions. It also yields a shorter operation time, thus improving the gate fidelity by limiting decoherence. This phase gate operation can be implemented in four steps, as illustrated in Table I.

First, we perform a formal two-qubit SWAP operation, by exchanging the labels of both molecules. We then transfer the rotational qubit  $|N=2\rangle$  of the ground vibrational level v=0 to the rotational state  $|N=1\rangle$  of the excited level v=1 using a short (ns)  $\pi$  pulse, as illustrated in Fig. 1.

The bandwidth of the pulse, much larger than the molecular dipole interaction energy, allows for the creation of the rotational wave packets

$$|10\rangle = (\Psi_2 - \Psi_3)/\sqrt{2},$$
  
 $|01\rangle = (\Psi_2 + \Psi_3)/\sqrt{2},$  (1)

from the storage qubits  $|20\rangle$  and  $|02\rangle$ .  $\Psi_2$  and  $\Psi_3$  denote here the eigenstates of the total bimolecular Hamiltonian defined in Eq. (9) of our original paper.

The wave packets (1) are then let to evolve freely during a duration  $\tau$ , yielding the quantum states

$$|10\rangle \rightarrow (e^{i\theta}\Psi_2 - e^{-i\theta}\Psi_3)/\sqrt{2},$$
  
$$|01\rangle \rightarrow (e^{i\theta}\Psi_2 + e^{-i\theta}\Psi_3)/\sqrt{2},$$
  
(2)

where  $\theta = \tau \Delta / \hbar$  with

$$\Delta = \frac{1}{6\pi\epsilon_0} \frac{\langle \mu \rangle^2}{r^3},\tag{3}$$

*r* being the intermolecular distance.

Here, the vibrational transition dipole moment  $\langle \mu \rangle$  between the states v=0 and v=1 is simply given by [1]

$$\langle \mu \rangle = \left(\frac{\partial \mu}{\partial R}\right)_{R_e} \sqrt{\frac{\hbar}{2m\omega_{\rm vib}}},\tag{4}$$

 $R_e$  being the equilibrium internuclear distance.

For  $\tau = \hbar \pi / 2\Delta$ , the states given in Eq. (2) turn into

$ 00\rangle$	$\stackrel{\text{SWAP}}{\longrightarrow}$	$ 00\rangle$	$\hbar \omega \longrightarrow$	$ 00\rangle$	$\stackrel{\text{dipole}}{\longrightarrow}$	$ 00\rangle$	$\hbar \omega \rightarrow$	$ 00\rangle$
$ 02\rangle$	$\rightarrow$	$ 20\rangle$	$\rightarrow$	$ 10\rangle$	$\rightarrow$	$i 01\rangle$	$\rightarrow$	$-i 02\rangle$
$ 20\rangle$	$\rightarrow$	$ 02\rangle$	$\rightarrow$	$ 01\rangle$	$\rightarrow$	$i 10\rangle$	$\rightarrow$	$-i 20\rangle$
22>	$\rightarrow$	$ 22\rangle$	$\rightarrow$	$ 11\rangle$	$\rightarrow$	$ 11\rangle$	$\rightarrow$	$ 22\rangle$

TABLE I. Operation of the proposed two-qubit  $\pi$  phase gate.



FIG. 1. (Color online) Schematic energy level diagram and excitation scheme.



FIG. 2. (Color online) (a) Gate duration  $\tau$  and (b) gate efficiency  $1/\gamma_{\rm vib}\tau$  as a function of the intermolecular separation  $r \simeq \lambda/2$  in an optical lattice of wavelength  $\lambda$ . The values corresponding to NaCs, LiCs, YbF, and BaF are shown.

$$|10\rangle \rightarrow i(\Psi_2 + \Psi_3)/\sqrt{2} = i|01\rangle,$$
  
$$|01\rangle \rightarrow i(\Psi_2 - \Psi_3)/\sqrt{2} = i|10\rangle.$$
 (5)

One can notice here that, for  $\tau = \hbar \pi / 2\Delta$ , exactly one unit of angular momentum  $\hbar$  has been exchanged between the two molecules. This effect is used here to create a maximally entangled state from a separable initial state. Indeed, the two initial bimolecular quantum wave packets  $|01\rangle$  and  $|10\rangle$  have been phase-shifted by  $\pi/2$ . This operation is conditional in the sense that it only affects molecules which differ by a single unit of angular momentum (see Table I).

In the last step, the initial states  $|0\rangle$  and  $|2\rangle$  are simply reestablished using a second  $\pi$  pulse identical to the one used in the excitation step. One ends up with a conditional two-qubit  $\pi$  phase gate (see Table I), performed in a duration

$$\tau = 4\pi\epsilon_0 \left(\frac{3\hbar\pi r^3}{4\langle\mu\rangle^2}\right).\tag{6}$$

Compared to expression (25) of our paper, the gate duration is reduced by a factor of 4, and the permanent dipole  $\mu$  is replaced by the average transition dipole given in Eq. (4).

The gate duration  $\tau$  and gate efficiency

$$1/\gamma_{\rm vib}\tau = \frac{1}{\pi} \left(\frac{c}{\omega_{\rm vib}r}\right)^3 \tag{7}$$

are shown in Figs. 2(a) and 2(b), respectively, for NaCs, LiCs, YbF and BaF.

One can notice in this figure that the shortest gate durations are obtained for the diatomic molecules YbF and BaF, which possess the largest permanent dipoles and the fastest variations of this dipole with the internuclear distance [1]. However, these molecules are not the ones yielding the best robustness [see Fig. 2(b)], since they are also associated with the largest vibrational frequencies.

<sup>[1]</sup> N. Vanhaecke and O. Dulieu, Mol. Phys. 105, 1723 (2007).