

High-fidelity molecular quantum logic gates resilient to interaction fluctuation

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Optically trapped polar molecules are promising for quantum information processing, yet the accuracy of an entangling molecular gate is limited by the uncertainty of dipole-dipole interactions (DDI) from the molecular motion in traps. We show that two π pulses of global microwave excitation can yield a spin-echo controlled-phase gate when assisted by two single-qubit gates, where the gate is resilient to the uncertainty of DDI because it strongly suppresses populating DDI-coupled states. Further, the controlled phase is fully tunable by varying the relative phase of the two global microwave pulses, and, hence, is applicable in a wide range of quantum algorithms involving quantum Fourier transform. We introduce a motional-mode separation technique to quantum mechanically study the influence of the molecular motion, which shows that the motion-induced infidelity of the gate can be below 0.0001 with typical experimental conditions.

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Polar molecules were proposed as candidates for building quantum information processing devices more than two decades ago [1], with multiple follow-up designs for molecular quantum entangling gates [2–8]. These gate protocols depend on shelving molecules transiently on a state coupled by dipole-dipole interaction (DDI), which can be either a state-dependent Ising-like energy shift [3,6] or a spin-exchange coupling [4,5,7,8]. Molecules are usually optically trapped during the logic operations, where the position spread inside the traps cannot be ignored compared to the molecule-molecule separation L [9–11], leading to an uncertainty of the DDI. Consequently, despite the remarkable advance of the cooling, trapping, and quantum state manipulation over ultracold polar molecules [12,13], experimental demonstrations of quantum entanglement [9–11,14,15] and two-qubit logic operations [10] revealed that the uncertainty of DDI strongly limits the gate accuracy. Recently, Ref. [7] proposed an optimal control scheme that can yield a two-molecule iSWAP gate with an infidelity below 2×10^{-4} with 10% variation of DDI.

Here, we introduce a way to realize a two-qubit molecular phase gate resilient to the uncertainty of DDI, and the gate is realized by two global microwave pulses when assisted by two single-qubit phase gates following each microwave pulse. Enabled by an exotic effective spin-echo process, the gate has two features. First, variation of DDI barely influences the gate accuracy due to that DDI serves as a channel to enable adiabatic dynamics where fine-tuning of DDI is no longer needed. Second, the entangling phase φ in the gate is from the global microwave field, so that φ can be of any desired value simply by tuning the relative phase between the microwave

pulses. Such a class of tunable controlled-phase gates can be used in quantum Fourier transform for notable quantum algorithms like phase estimation, order-finding, and the Shor's algorithm [16].

We introduce a theory to quantum mechanically study the influence of the molecular motion in the trap on the entangling gate. When neglecting the much weaker motion along the radial direction in typical tweezers, the molecular motion along the axial directions results in a coupling between the two molecules' harmonic motional modes and the DDI-coupled internal states. Quantum mechanically, this means that two motional modes are coupled to the internal states of the molecules via DDI. By a motional-mode separation technique, however, we find that though there are two modes involved in the molecular motion, only one is coupled to the internal state of the molecules. By this formalism, we find that the error from the quantized motion of the two-qubit phase gate can be below 0.0001 with typical molecular motion in traps of recent experiments [9,10].

A controlled-phase gate by an effective spin echo. For two molecules, labeled i and ii, we consider three different states $|\uparrow\rangle$, $|\downarrow\rangle$, and $|e\rangle$ for each molecule, where the former two are qubit states and the last is a state coupled to $|\downarrow\rangle$ via a microwave field of a Hamiltonian $\hat{H}_\mu = \hbar\Omega_\mu(t)|e\rangle\langle\downarrow|/2 + \text{H.c.}$, which is in a rotating frame after performing dipole and rotating-wave approximations. Since the microwave field in use has a wavelength on the order of decimeter, while the molecular separation is on the order of micrometer, the same microwave field covers both molecules with equal strength and phase. In the Hilbert space spanned by the states of the two molecules, the microwave driving for the two molecules induces a Hamiltonian $\hat{H}_\mu \otimes \hat{I} + \hat{I} \otimes \hat{H}_\mu$, with $\hat{I}$ the identity operator. To induce entanglement, we consider a condition without applying static electric field and that a two-molecule state in a superposition of $|\uparrow e\rangle$ of $|e\uparrow\rangle$ experiences a dipole-dipole interaction $\hat{V} = \mathcal{J}(|\uparrow e\rangle\langle e\uparrow| + |e\uparrow\rangle\langle\uparrow e|)$ [4], where $\mathcal{J}$ denotes the DDI with motion-induced fluctuation. The absence of DDI in $|\downarrow\rangle$ can be realized by selection rule

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or that an electric DDI does not change nuclear spin states [6,10,17]. A useful example is in Ref. [10], where the nuclear spin states in $|e\rangle$ and $|\downarrow\rangle$ differ [18], but a weakly allowed quadrupole transition is realized with a Rabi frequency about $2\pi \times 1.6$ kHz. Because DDI is dipole driven, the quadrupole moment between $|e\rangle$ and $|\downarrow\rangle$ does not enter the DDI. For the gate here, it should be better to choose controllable states not based on state mixing from magnetic or tweezer fields because external-field-induced transition $|e\rangle \leftrightarrow |\downarrow\rangle$ would open a weak DDI channel $|\downarrow e\rangle \leftrightarrow |e\downarrow\rangle$.

In the context of quantum logic gates, it is useful to study the gate map by examining the time dynamics for the energy eigenstates of the gate [19,20], which are $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ here. The microwave field only couples $|e\rangle$ and $|\downarrow\rangle$, so the state $|\uparrow\uparrow\rangle$ stays intact in the rotating frame. Both $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ are coupled by the microwave field, with dynamics that can be conveniently described by $\hat{H} = \hat{H}_+ + \hat{H}_-$, with

$$\hat{H}_{\pm} = \left[\hbar \frac{\Omega_{\mu}(t)}{2} |\mathbb{D}_{\pm}\rangle \langle \mathbb{B}_{\pm}| + \text{H.c.} \right] \pm \mathcal{J} |\mathbb{D}_{\pm}\rangle \langle \mathbb{D}_{\pm}|,$$

and $\mathbb{D}$ and $\mathbb{B}$ are DDI-coupled Bell states and qubit-space Bell states, given by $|\mathbb{D}_{\pm}\rangle = \frac{1}{\sqrt{2}}(|\uparrow e\rangle \pm |e\uparrow\rangle)$ and $|\mathbb{B}_{\pm}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$, respectively. Here, the use of Bell-state basis does not mean that the gate works in Bell-state basis. It is used only for showing the gate mechanism, and the numerical results are from the original Hamiltonian without use of any Bell-state basis.

In a classical picture, $\mathcal{J}$ is fluctuating or uncertain due to the molecular motion in the optical trap, so that any control scheme by a microwave driving will be subjected to a control error. To remove this error, we introduce an adiabatic spin-echo sequence by noting that $\hat{H}_{\alpha}$ is equivalent to $\hat{H}_{\alpha} = \sum_{\eta=\pm} \xi_{\eta}^{(\alpha)} |v_{\eta}^{(\alpha)}\rangle \langle v_{\eta}^{(\alpha)}|$, with $\xi_{\eta}^{(\alpha)} = (\alpha \mathcal{J} + \eta \hbar \bar{\Omega}_{\mu})/2$ and $|v_{\eta}^{(\alpha)}\rangle = [\xi_{\eta}^{(\alpha)} |\mathbb{D}_{\alpha}\rangle + \hbar \Omega_{\mu}^*(t) |\mathbb{B}_{\alpha}\rangle / 2] / \mathcal{N}_{\eta}^{(\alpha)}$, where $\bar{\Omega}_{\mu} = [\mathcal{J}^2 / \hbar^2 + |\Omega_{\mu}|^2]^{1/2}$ and $\mathcal{N}_{\eta}^{(\alpha)} = [|\xi_{\eta}^{(\alpha)}|^2 + \hbar^2 |\Omega_{\mu}(t)|^2 / 4]^{1/2}$. When $\Omega_{\mu} = 0$ at $t = 0$ and $\mathcal{J} < 0$, we have $|\mathbb{B}_{+}\rangle = |v_{+}^{(+)}\rangle$ and $|\mathbb{B}_{-}\rangle = |v_{-}^{(-)}\rangle$ (Supplemental Material Ref. [21]), and when we smoothly ramp up the microwave Rabi frequency to a maximum Ω , and then back to zero again, we have

$$|\mathbb{B}_{\pm}\rangle \rightarrow e^{\mp i\phi} |\mathbb{B}_{\pm}\rangle, \quad (1)$$

where $\phi = \int_0^T \xi_{+}^{(+)} dt / \hbar$ with the relation $\xi_{+}^{(+)} = -\xi_{-}^{(-)}$.

After the first π pulse, a phase gate that imprints a π phase to the $|\downarrow\rangle$ state of molecule i is applied. This operation needs single-site addressing, as in Ref. [7], and can be realized by ac Stark shift via trap-depth control [14], trap-depth control and state shelving [10,25], level shifting by laser fields [26], or two-photon Raman transition [17]. As detailed in Ref. [21], three among these four methods are more suitable for realizing the required site-selective phase operations, with infidelity of the gate in the range $(9, 17) \times 10^{-5}$ accounting for intrinsic undesired state dynamics and decoherence of the qubit states. To have faster gates, the method of using optical Raman transition as in Ref. [17] is more favorable, with gate time about $t_{\text{phase}} = 67 \mu\text{s}$ realizable because a two-photon Rabi frequency $\Omega_R \approx 2\pi \times 15$ kHz was demonstrated [17].

With the phase gate at hand, it induces

$$|\mathbb{B}_{\pm}\rangle \rightarrow |\mathbb{B}_{\mp}\rangle, \quad (2)$$

where nothing occurs to the input state $|\downarrow\downarrow\rangle$ because it is $-|ee\rangle$ due to the already-applied first microwave pulse.

Then, a second π pulse of microwave field with Rabi frequency $e^{-i(\pi+\varphi)/2} \Omega_{\mu}(t)$ is sent to the molecules. According to the adiabatic picture, we again have the state evolution as in Eq. (1). Note that the phase shift to the microwave field does not alter the adiabatic picture. The only effect of this phase change is that the input state $|\downarrow\downarrow\rangle$, which is $-|ee\rangle$ at the beginning of the second microwave pulse, will have an extra phase shift $\varphi + \pi$ when it returns back to the ground state. Then, the state evolution from the first microwave pulse to the end of the second microwave pulse is

$$|\mathbb{B}_{\pm}\rangle \rightarrow |\mathbb{B}_{\mp}\rangle, \quad |\downarrow\downarrow\rangle \rightarrow -e^{i\varphi} |\downarrow\downarrow\rangle. \quad (3)$$

Finally, we use the phase shift gate as used for Eq. (2). The phase shift π to the $|\downarrow\rangle$ state of molecule i also imprints a π phase to $|\downarrow\downarrow\rangle$. As a consequence, the net effect for the two global microwave pulses and two single-qubit phase gates is $|\downarrow\downarrow\rangle \mapsto e^{i\varphi} |\downarrow\downarrow\rangle$, while all the other state components remain unchanged. For $\varphi = \pm\pi$, the gate is the CZ gate that can be transformed to a controlled-NOT gate via single-qubit rotations [27].

To examine how much can the adiabatic picture tolerate a moderate $|\mathcal{J}|/(\hbar\Omega)$, we take, as an example,

$$\Omega_{\mu}(t) = \Omega \left[e^{-\frac{(t-T/2)^2}{2t_w^2}} - e^{-\frac{T^2}{8t_w^2}} \right], \quad \text{when } t \leq T,$$

$$\Omega_{\mu}(t) = \Omega_{\mu}(t - T), \quad \text{when } t \in t_{\text{phase}} + (T, 2T], \quad (4)$$

and set $t_w = 0.234T$ at which $\Omega \approx 6.75/T$ is smallest, while simultaneously satisfies $\int_0^T \Omega_{\mu} dt = \pi$, where t_{phase} is the duration of the single-qubit phase gate to molecule i. With the pulse of Eq. (4) and a Hamiltonian in the basis of $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, \dots\}$, Fig. 1 shows the numerically evaluated conditioned infidelity $\mathcal{E}$ of the gate with the definition of fidelity from Ref. [28], where “conditioned” means that $\mathcal{E}$ includes neither decoherence of the two-qubit states nor technique noise. The infidelity in Fig. 1 comes from diabatic leakage.

Influence from position spread in traps. The trap frequencies along the axial and radial directions differ by one order of magnitude in usual experimental setups [9], enabling the neglect of the motion along the two radial directions. We can consider the centers for two traps at $(0, 0, 0)$ and $(0, L, 0)$, with the axial direction along $\mathbf{x}$. Along the axial direction, the Hamiltonian for the two trapped molecules is $\hat{H}_{\text{trap}} = \sum_{\alpha=i,ii} [p_{\alpha}^2/(2m) + m\omega^2 x_{\alpha}^2/2]$, where $\alpha = i, ii$, ω is the angular frequency along the axial direction, m is the mass of the molecule, and $p_{\alpha} = -i\hbar\partial/\partial x_{\alpha}$. To capture the coupling between the external motion and the internal rovibrational states, we define

$$x_{\pm} = (x_i \pm x_{ii})/\sqrt{2}, \quad p_{\pm} = -i\hbar\partial/\partial x_{\pm}, \quad (5)$$

so that $\hat{H}_{\text{trap}} = \sum_{\alpha=\pm} [p_{\alpha}^2/(2m) + m\omega^2 x_{\alpha}^2/2]$, which means that the state of the external two-molecule vibration in the two-trap system is a product state of the two motional modes labeled $\pm$. The wavefunctions of the ground and the n th-excited two-trap motional state of the molecules

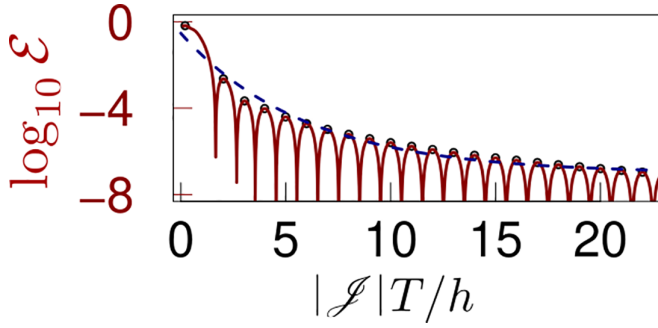


FIG. 1. The solid curve shows $\log_{10}(\text{conditioned infidelity})$ of the CZ gate, i.e., a two-qubit gate with a controlled phase $\varphi = \pi$, simulated with the pulse in Eq. (4); here “conditioned” means that $\mathcal{E}$ includes neither decoherence of the two-qubit states nor technique noise, but only accounts for the intrinsic rotation errors as compared to the desired adiabaticity. Here, the oscillation of the infidelity when varying J arises from the detuned nature of the Rabi cycles, which is a common feature in detuned Rabi oscillation [23]. The small circles denote local maximal, to which the dashed curve shows a fit with $\log_{10}\mathcal{E} = 6.49\exp(-0.168|J|T/h) - 7.02$. The decay of $\mathcal{E}$ indicates weaker diabatic leakage with longer pulses.

are $|0_\alpha\rangle \equiv |\text{vac}_\alpha\rangle$ and $|n_\alpha\rangle$, with $n = 1, 2, \dots$. Here, $|n_\alpha\rangle = \frac{1}{\sqrt{2^n n! \ell \sqrt{\pi}}} e^{-\frac{x_\alpha^2}{2\ell^2}} h_n(x/\ell)$, $\ell = \sqrt{\hbar/(m\omega)}$, and the Hermitian polynomials $h_n(\xi)$ are given by $h_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}$, which is an eigenstate of eigenenergy $E_n = \frac{1}{2}\hbar\omega(2n+1)$. In the Hilbert space spanned by $|n_\alpha\rangle$, the motional Hamiltonian is $\hat{H}_{\text{trap}} = \hbar\omega \sum_{\alpha=\pm} (\hat{a}_\alpha^\dagger \hat{a}_\alpha + 1/2)$, where $\hat{a}_\alpha^\dagger$ and $\hat{a}_\alpha$ are the creation and annihilation operators for the motional states of the two-molecule motional mode $\alpha = +$ or $-$, which is related to x_α via $x_\alpha = (\hat{a}_\alpha^\dagger + \hat{a}_\alpha)\ell/\sqrt{2}$. Then, the modes $\pm$ are related to the modes i and ii via $\hat{a}_\pm = (\hat{a}_i \pm \hat{a}_{ii})/\sqrt{2}$ and similarly for the creation operator $\hat{a}_\pm^\dagger$. So, if the two molecules are both in the motional ground states, the state in the basis of $\alpha = \pm$ is also the ground one.

The motional-mode separation in Eq. (5) is useful for studying the coupling between DDI and molecular motion in the traps. As shown in the Supplemental Material [21], when the quantization axis is along y , the coupling strength of the DDI can be written as

$$J \approx J_0 \left[\frac{3\ell^2}{L^2} (\hat{a}_-^\dagger + \hat{a}_-)^2 - \frac{45\ell^4}{8L^4} (\hat{a}_-^\dagger + \hat{a}_-)^4 - 1 \right], \quad (6)$$

which shows that the DDI only couples with the $\hat{a}_-$ mode, where J_0 is the strength of DDI when each molecule is at the center of the corresponding trap. In other words, even if the two-trap motional state of the $\hat{a}_+$ mode is highly excited, it still has no influence on the DDI since only the $\hat{a}_-$ mode is involved.

In a recent experiment reported in Ref. [9], the molecules in the traps were in the ground and the first excited states, with little chance to be in a higher state. When converting from the original modes to the $\hat{a}_\pm$ mode, one can see that the frequencies for the four modes are equal. In other words, if we assume that the molecules are cooled to states with no more than one motional quantum, then the worst case in the relevant $\hat{a}_-$ mode is that we have one vibration quantum in it.

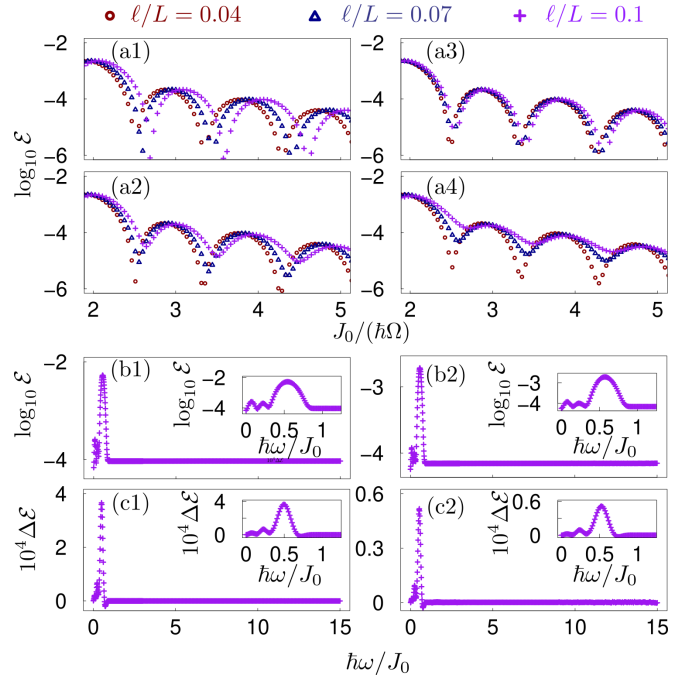


FIG. 2. (a1)–(a4) Round, triangle, and cross symbols show $\log_{10}\mathcal{E}$ of the CZ gate, with $\ell/L = 0.04, 0.07$, and 0.1 , respectively, where J_0 is the DDI when molecules are exactly at the centers of the corresponding traps. Here, ℓ is the harmonic oscillator length and L the distance between the centers of the two tweezers. The initial states for the $\hat{a}_-$ mode of the motion are $\hat{a}_-^\dagger|\text{vac}_-\rangle$, $(1 + \hat{a}_-^\dagger)|\text{vac}_-\rangle/\sqrt{2}$, and $|\text{vac}_-\rangle$ in panels (a1), (a2), and (a3), respectively. The initial state in panel (a4) is a thermal state with $\langle \hat{a}_-^\dagger \hat{a}_- \rangle = 2$. Parameters are the same as those in Fig. 1, except that here we need another parameter, i.e., the trap frequency, for which we set $\hbar\omega = 13.4J_0$ because J_0 and the axial trap frequency in Ref. [10] are 0.37 and 4.95 kHz, respectively [29]. Panels (b1) and (b2) show $\log_{10}\mathcal{E}$ as a function of trap frequency with $J_0 = 3\Omega$ and $\ell/L = 0.1$, with $\hat{a}_-^\dagger|\text{vac}_-\rangle$ and $|\text{vac}_-\rangle$ the initial motional states. One can see that there is a trap-dipole resonance around $\hbar\omega = 0.5J_0$, as studied in Ref. [29]. Panels (c1) and (c2) show the difference between $\mathcal{E}$ via the full DDI operator and $\mathcal{E}$ via the truncated DDI in Eq. (6) with corresponding parameters of panels (b1) and (b2), respectively. The error due to the truncation of DDI is on the order of 10^{-4} around the trap-dipole resonance, but reduces to zero away from the resonance. The insets in panels (b1), (b2), (c1), and (c2) show the close-up around the trap-dipole resonance. Here, states up to 40 motional excitations of the $\hat{a}_-$ mode are included in the simulation via QuTip [30,31], at which we find the simulation converged to a high level; we found no difference between results with 40 motional excitations and those with 100 motional excitations. Due to the finite pulse duration, the diabatic leakage shown in Fig. 1 is intrinsically incorporated.

The major influence from the motional states is that states with more motional excitations contribute more to the change of motional states, which is detrimental because it results in undesired entanglement between the external motion and the internal states. For analyzing the gate fidelity, we take both pure and thermal motional states. With $\hbar\omega/J_0 = 13.4$ [10], Figs. 2(a1)–2(a3) show the conditional infidelity $\mathcal{E}$ with three representative pure motional states $\hat{a}_-^\dagger|\text{vac}_-\rangle \otimes |A_+\rangle$, $[(1 + \hat{a}_-^\dagger)|\text{vac}_-\rangle/\sqrt{2}] \otimes |A_+\rangle$, and $|\text{vac}_-\rangle \otimes |A_+\rangle$, respectively,

with $|A_+\rangle$ an arbitrary state for the $\hat{a}_+$ mode of the motion. Figures 2(b1), 2(b2), 2(c1), and 2(c2) show that the truncated DDI in Eq. (6) is a useful approximation when trap-dipole resonance [29] is avoided. The evaluation of $\mathcal{E}$ is based on extracting the input-output coefficient when including the motional state. In case of thermal motional state, we can take the off-diagonal matrix block with coherence between the nonevolved internal state and the evolved one, and then trace the inner product between the extracted matrix block and the initial motional state. This allows one to extract the relevant input-output coefficient of the involved state component [21]. Figure 2(a4) shows results when the initial motion is a thermal state with $\langle \hat{a}_+^\dagger \hat{a}_+ \rangle = 2$. With $J_0 = h \times 0.37$ kHz from $L = 1.79 \mu\text{m}$ of Ref. [10], the duration of the two adiabatic pulses is $2T \approx 17$ ms if $J_0/(\hbar\Omega) = 3$, at which $\mathcal{E}$ is below 2×10^{-4} in the four cases of Figs. 2(a1)–2(a4) when $\ell/L = 0.04$, which is near to the condition of Ref. [10]. If we consider trap-depth control and state shelving for realizing the site-selective single-qubit phase gate, the duration of two such single-qubit gates can be about 3 ms, while the total error of them can be about $2\mathcal{E}_s \approx 1.8 \times 10^{-4}$, as shown in Sec. II B of Ref. [21]. In case of trapping the molecules in optical tweezers formed from light at a magic wavelength as in Ref. [9], T_2^* of the qubits can be over 15 s, so that the infidelity of the full controlled-phase operation $\mathcal{E} + 2T/T_2^* + 2\mathcal{E}_s$ is below 0.0015 if $J_0/(\hbar\Omega) = 3$ in Figs. 2(a1)–2(a4).

Other effects. It is useful to estimate the impact of the radial motion that is neglected above. The trap frequencies along the radial and axial directions usually differ by one order of magnitude or more. For example, they are 3.0 and 0.4 kHz in Ref. [9], respectively, and Ref. [10] stated that only the motion along the axial direction matters. If the radial ω_r is 10 times larger than the axial ω , then ℓ_r along the radial direction is $\sqrt{10}$ times smaller. There are two orthogonal radial modes, so the extra error due to the motion along the two radial directions should be $2\Delta\mathcal{E}(\ell_r)$, with $\Delta\mathcal{E}(\ell_r)$ given by the simulated infidelity deducted by the one simulated as in Fig. 1 because the latter takes into account the nonadiabatic effect. By the same simulation as in Fig. 2(a4), we have $\Delta\mathcal{E}(\ell_r) \approx (2.6, 7.8, 15.2) \times 10^{-6}$, with $\ell_r = (0.04, 0.07, 0.1)L/\sqrt{10}$ when $J_0/(\hbar\Omega) = 3$. This means that the neglected radial motion is marginal.

Another noise is that there can be certain uncertainty of the trap centers, leading to shot-to-shot variation of J_0 with respect to the desired value. One can average $\mathcal{E}$ by J_0 over, e.g., $[3, 5]\hbar\Omega$, i.e., a 25% change if $4\hbar\Omega$ is desired, with results shown in Table I. For the experiments in Ref. [10], $\ell \approx 0.1 \mu\text{m}$ and $L \in [1.79, 2.5] \mu\text{m}$, yielding $\ell/L \in (0.04, 0.06)$. Remarkably, the infidelity with a thermal motional state of $\langle \hat{a}_+^\dagger \hat{a}_+ \rangle = 2$ is slightly smaller than that with a pure state $\hat{a}_+^\dagger |\text{vac}_+\rangle$ when $\ell/L = 0.07$ or 0.1. According to Table I, the influence of the coupling to motional states, with $\ell/L \in (0.04, 0.06)$, is weak.

The example shown in Figs. 1, 2, and Table I reveals that if $\ell/L = 0.04$ near the condition of Ref. [10], we have $\mathcal{E} < 0.0001$ even if the molecules are in a thermal state of the $\hat{a}_-$ mode with two motional quanta. In Ref. [9], about

TABLE I. Average conditional infidelity with J_0 equally sampled over $[3, 5]\hbar\Omega$ for three representative pure initial states of the $\hat{a}_-$ motional mode, and a thermal initial state with two motional quanta in the $\hat{a}_-$ mode. Other parameters are adopted from Fig. 2.

$\hat{a}_-$ state $\backslash \ell/L$	0.04	0.07	0.1
$\hat{a}_+^\dagger \text{vac}_+\rangle$	4.33×10^{-5}	5.15×10^{-5}	6.31×10^{-5}
$(1 + \hat{a}_+^\dagger) \text{vac}_+\rangle / \sqrt{2}$	4.21×10^{-5}	4.74×10^{-5}	5.53×10^{-5}
$ \text{vac}_+\rangle$	4.05×10^{-5}	4.31×10^{-5}	4.71×10^{-5}
Thermal, $\langle \hat{a}_+^\dagger \hat{a}_+ \rangle = 2$	4.37×10^{-5}	5.02×10^{-5}	5.81×10^{-5}

58% of molecules occupy the motional ground state, and most of the motional excited molecules have just one motional quantum. In practice, it is not trivial to have the molecules in a pure motional state, so that it is possible that the results in Fig. 2(a4) are more practical. This means that the adiabatic gate can strongly suppress the motion-induced error with currently available experimental conditions.

Discussion and conclusions. The gate here is analogous to dark-state gates in Rydberg atoms (for a review, see, e.g., Ref. [27]). One difference from Rydberg atoms is that the dark-state gates with Rydberg atoms need to populate multiple Rydberg states that have lifetimes of order of 0.1 ms, but DDI occurs between molecules in low-lying states. Here, $|\uparrow\rangle$ and $|\downarrow\rangle$ can be in the ground rovibrational manifold and $|e\rangle$ in the first excited manifold, all possessing long lifetimes. A particular strength of polar molecules is that it is possible to trap multiple low-lying states in the same trap with second scale coherence, while simultaneously enabling coherent state transitions between the states [32]. This can enable high-fidelity controlled-phase gates with polar molecules.

In summary, we introduce a controlled-phase gate with two polar molecules implemented by two adiabatic π pulses of microwave fields assisted by two single-qubit phase gates. The gate acquires a fully tunable phase determined by the phase change from the first to the second microwave pulses. We further introduce a quantum mechanical treatment to analyze the molecular motion in the trap and find that the gate infidelity from the molecular motion can be below 0.0001 with recent experimental setups.

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Data availability. There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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