Strong atom–field coupling for Bose–Einstein condensates in an optical cavity on a chip

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Supplementary Notes

1   Conditions for collective interaction

This section summarizes some facts about collective interaction of N two-level atoms with a single mode of the radiation field in the strong-coupling regime.

Let us first consider N atoms at fixed positions, all identically coupled to a single mode of the radiation field [S1] with a coupling strength g_1. We call $|g_i\rangle$ and $|e_i\rangle$ the ground and excited internal states of the ith atom. If initially all atoms are in the ground state $|\Psi_0\rangle = |g \dots g\rangle$ and then the system is weakly excited, the first excited state must reflect the symmetry of the situation and therefore is [S2]

$$|\Psi_1\rangle = \frac{1}{\sqrt{N}} \left(|e, g \dots g\rangle + |g, e, g \dots g\rangle + \dots + |g \dots g, e\rangle\right) . \tag{1}$$

The coupling term in the Hamiltonian, setting $\hbar = 1$, is

$$\widehat{V} = g_1 \left(\sum_i \hat{a} |e_i\rangle \langle g_i| \right) + \text{h.c.} , \tag{2}$$

where $\hat{a}$ annihilates one photon in the mode. The matrix element g_N between the atomic ground state with one photon in the field mode, $|1\rangle \otimes |\Psi_0\rangle$, and the atomic first excited state with no photon, $|0\rangle \otimes |\Psi_1\rangle$, is therefore

$$g_N = \langle 0| \otimes \langle \Psi_1| \widehat{V} |\Psi_0\rangle \otimes |1\rangle = \sqrt{N} g_1 . \tag{3}$$

The atomic ensemble thus behaves as a single "superatom", with a collective enhancement $\sqrt{N}$ in the coupling strength.

No assumption about the particle statistics was made to obtain this result. However identical coupling was assumed, which in a real experiment is strictly true only for a Bose–Einstein condensate (BEC), where all atoms share the same spatial wavefunction. In the following we show that even for nonidentical couplings the atomic ensemble interacting with the cavity field can be described as a two-level system, and that the $\sqrt{N}$ scaling of the collective coupling strength still holds. The main result is that $g_N = \sqrt{N}\bar{g}_1$ with $\bar{g}_1^2 = \int \frac{\rho(\mathbf{r})}{N} |g_1(\mathbf{r})|^2 d\mathbf{r}$, where $g_1(\mathbf{r})$ is the position-dependent single-atom coupling strength to the field mode and $\rho(\mathbf{r})$ is the atomic density distribution. Additionally, the reasoning below does not make the approximation of point-like atoms, so that it applies to laser-cooled atoms and BECs for which the size of the atomic wavefunction can easily exceed the optical wavelength (note that the demonstration would be much simpler using the point-like approximation). The case of a *single* atom with quantized motion was considered by Vernooy and Kimble [S3], who

1

found complex dynamics with collapses and revivals of the Rabi oscillations between the ground and excited states of the atom.

The complete (neglecting damping) N atoms–field Hamiltonian in a cavity can be written

$$\widehat{H} = \underbrace{\omega_C\,\hat{a}^\dagger\hat{a} + \omega_A \sum_{i=1}^N \hat{\sigma}_i^\dagger\hat{\sigma}_i}_{\widehat{H}_0} + \underbrace{\sum_{i=1}^N \left(g_1(\hat{\mathbf{r}}_i)\,\hat{a}\hat{\sigma}_i^\dagger + g_1^*(\hat{\mathbf{r}}_i)\,\hat{a}^\dagger\hat{\sigma}_i \right)}_{\widehat{V}}, \tag{4}$$

where $\hat{\sigma}_i$ is the atomic lowering operator $\hat{\sigma}_i = |\mathrm{g}_i\rangle\langle\mathrm{e}_i|$ and $\hat{a}$ the cavity photon destruction operator. The kinetic energy of the atoms is neglected, which is valid as long as the broad line condition $E_{\mathrm{rec}} \ll \hbar\Gamma$ applies, meaning that a few recoil kicks will not drive the atoms out of resonance (see for example [S4]).

Suppose that the atom–cavity compound system is initially is the stationary state $|G\rangle \equiv |0;\mathrm{g}\ldots\mathrm{g};\Phi\rangle$: no photon is in the cavity, all the atoms are in the internal ground state $|\mathrm{g}\rangle$ and their positions are described by a N-particle wavefunction $|\Phi\rangle$. When the cavity is pumped, the system can undergo transitions to the first excited state $|E_1\rangle \equiv |1;\mathrm{g}\ldots\mathrm{g};\Phi\rangle$. This level is coupled via $\widehat{V}$ to a second excited state $|E_2\rangle$ defined by:

$$|E_2\rangle = \widehat{V}|E_1\rangle = |0\rangle \otimes \sum_i |\mathrm{g}\ldots \underbrace{\mathrm{e}}_{i^{th}\,term} \ldots\mathrm{g}\rangle \otimes g_1(\hat{\mathbf{r}}_i)|\Phi\rangle \tag{5}$$

up to a normalization constant. To confirm that the atomic ensemble interacting with the cavity field behaves like a two-level system, one has to show that the action of $\widehat{V}$ on $|E_2\rangle$ is mainly a coupling to $|E_1\rangle$. Therefore one has to compute

$$\widehat{V}|E_2\rangle = |1;\mathrm{g}\ldots\mathrm{g}\rangle \otimes \sum_i |g_1(\hat{\mathbf{r}}_i)|^2|\Phi\rangle. \tag{6}$$

When the two-particle position correlations are small, as in a classical gas or in a Bose–Einstein condensate, one can show that the final position wavefunction differs only slightly from the initial one:

$$\sum_i |g_1(\hat{\mathbf{r}}_i)|^2|\Phi\rangle = \left(\sum_i \langle |g_1(\hat{\mathbf{r}}_i)|^2 \rangle_\Phi \right) \left(|\Phi\rangle + \mathcal{O}(\frac{1}{\sqrt{N}}) \right) = g_N^2|\Phi\rangle + \mathcal{O}(\sqrt{N}), \tag{7}$$

$< \cdot >_\Phi$ standing for the quantum average (expectation value) in the state $|\Phi\rangle$. This would not be true for a quantum state presenting strong correlations, such as a Schrödinger cat, for which the position of the atoms would become highly entangled with the internal state.

Finally, the coupling $\widehat{V}$ can be rewritten as the sum of a two-level coupling $\widehat{V}_{JC}$, and a many-level coupling term $\widehat{V}'$ of smaller magnitude, which corresponds to cloud heating and spreading on a longer timescale due to interaction with the cavity field. The two-level coupling can be cast in the familiar Jaynes–Cummings form $\widehat{V}_{JC} = g_N(\hat{a}\hat{\sigma}^\dagger + \hat{a}^\dagger\hat{\sigma})$ with an effective, scalar coupling strength g_N scaling as $\sqrt{N}$, as in the case of identically coupled point-like atoms (3):

$$g_N^2 = \sum_{i=1}^N \langle |g_1(\hat{\mathbf{r}}_i)|^2 \rangle_\Phi = N \langle |g_1(\hat{\mathbf{r}}_i)|^2 \rangle_{\Phi,i} = \int \langle \hat{\rho}(\mathbf{r}) \rangle_\Phi\, |g_1(\mathbf{r})|^2 \mathrm{d}\mathbf{r}, \tag{8}$$

and hence

$$g_N = \sqrt{N}\bar{g}_1, \text{ with } \bar{g}_1^2 = \int \frac{\rho(\mathbf{r})}{N}|g_1(\mathbf{r})|^2 \mathrm{d}\mathbf{r}. \tag{9}$$

2

2 Multilevel coupling model

In our experiments, ^{87}Rb atoms are trapped in the $|F = 2\rangle$ hyperfine level of the $5S_{1/2}$ ground state. We note $\Delta_{\mathrm{L}} = \omega_{\mathrm{L}} - \omega_{\mathrm{A}}$ the detuning of the probe beam relative to the $5S_{1/2} |F = 2\rangle \rightarrow 5P_{3/2} |F' = 3\rangle$ line of the D_2 transition. When $|\Delta_{\mathrm{L}}|$ exceeds the $\sim 500\,\mathrm{MHz}$ hyperfine splitting of the $5P_{3/2}$ excited state, one can treat the $5S_{1/2} |F = 2\rangle \rightarrow 5P_{3/2} |F' = 1, 2, 3\rangle$ transitions as a whole, which allows a two-level approach for the atoms. However, at the very large atoms–cavity coupling strengths reached in the experiment, additional atomic levels may play a role in the coupled system. In particular, when the coupling g_N is of the order of the hyperfine splitting of the $5S_{1/2}$ ground state $\Delta_{\mathrm{HFS}} = (E_{F=2} - E_{F=1})/\hbar \approx 2\pi \times 6.8\,\mathrm{GHz}$, the transitions $|F = 1\rangle \rightarrow 5P_{3/2}$ and $|F = 2\rangle \rightarrow |\mathrm{upper\ dressed\ state}\rangle$ may become simultaneously resonant with the probe field. As we will see, this leads to new features in the spectrum provided that the $|F = 1\rangle$ state is populated, even by a small fraction of atoms.
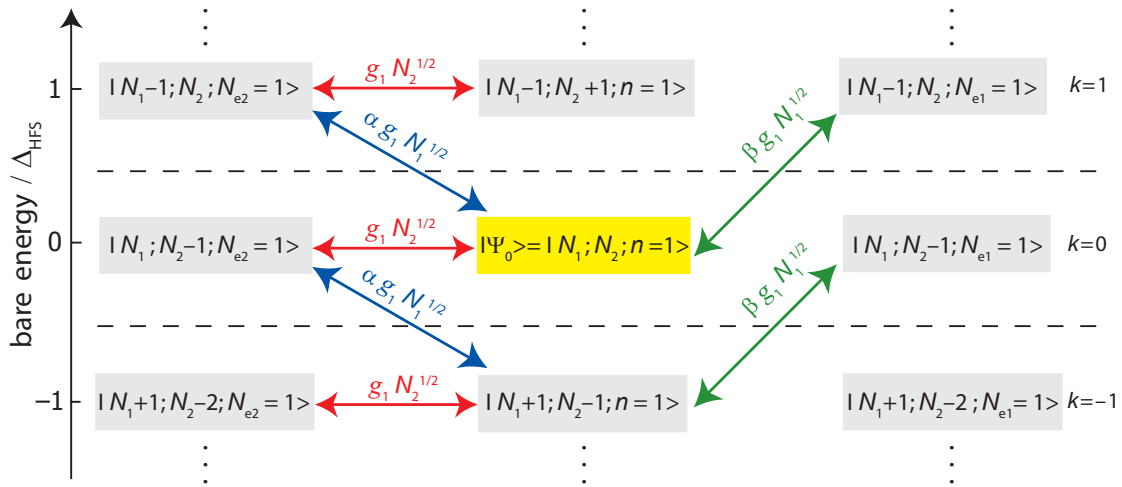

Supplementary figure 1: Outline of the first-excited states involved in the calculation of the cavity transmission spectrum. Left and right column states are "atom-like" (they contain one excited atom), central column states are "cavity-like" (they contain one photon). The vertical axis is the bare energy, in units of the ground state hyperfine splitting Δ_{HFS}. The initial state $|\Psi_0\rangle$ is in the centre. Horizontal and oblique arrows indicate the coupling strengths. The dashed lines separate the k subspaces; we restrict the graph to $k = -1, 0, 1$ for clarity. The cavity is tuned on the $5S_{1/2} |F = 2\rangle \rightarrow 5P_{3/2}$ transition, as in the experiment of Fig. 3a (main text).

A simple model taking into account this new transition is a four-level atom, with ground states $|g_{1,2}\rangle \equiv 5S_{1/2} |F = 1, 2\rangle$ of energies $-\hbar\Delta_{\mathrm{HFS}}$ and 0, and excited states $|e_{1,2}\rangle$ of energy $\hbar\omega_{\mathrm{A}}$. The cavity coupling can be developed on this basis (in the rotating wave approximation):

$$\widehat{V}_1 = \widehat{\mathbf{D}} \cdot \widehat{\mathbf{E}} = \hbar g_1 \,\hat{a} \Big(|e_1\rangle\langle g_2| + \alpha |e_1\rangle\langle g_1| + \beta |e_2\rangle\langle g_1| \Big) + \mathrm{h.c.} \tag{10}$$

in which the parameters $\alpha, \beta \lesssim 1$ depend on the polarization of the cavity field. A generic state for the N-atoms + cavity system is described by the number of atoms in each state and the number of photons in the cavity: $|\Psi\rangle = |N_{g_1}; N_{g_2}; N_{e_1}; N_{e_2}; n\rangle$. The initial state is $|N_1; N_2; 0; 0; 0\rangle$, where it is hypothesized that a relatively small number of atoms $N_1 \ll N_2$ are in the $|F = 1\rangle$ state. When the cavity is weakly pumped with the probe laser, the system is excited to the "cavity-like" state $|\Psi_0\rangle \equiv |N_1; N_2; 0; 0; 1\rangle$. This level is coupled to many other states with the same number of excitations $M = N_{e_1} + N_{e_2} + n = 1$, which we write $|N_1 - k; N_2 + k - N_{\mathrm{e}}; N_{e_1}; N_{e_2}; n\rangle$, with $N_{\mathrm{e}} = N_{e_1} + N_{e_2}$ and k an integer (Supplementary figure 1). For growing $|k|$ values, these levels of energy $\sim k \times \hbar\Delta_{\mathrm{HFS}}$ get progressively out of resonance with $|\Psi_0\rangle$. We thus restrict $|k|$ to small values, $k = -3 \ldots 3$, and diagonalize the coupling in this 3×7 - dimensional subspace. Each eigenenergy E is related to a peak in the frequency spectrum at a detuning $\delta \equiv (E - E_{\Psi_0})/\hbar = \omega_{\mathrm{L}} - \omega_{\mathrm{C}}$, with a weight $\sim |\langle\Psi|\Psi_0\rangle|^2$.

When the cavity is tuned on the $5S_{1/2} |F = 2\rangle \rightarrow 5P_{3/2}$ transition ($\Delta_{\mathrm{C}} = 0$), the model predicts an anticrossing in the positive part of the spectrum ($\delta > 0$) when the double resonance condition

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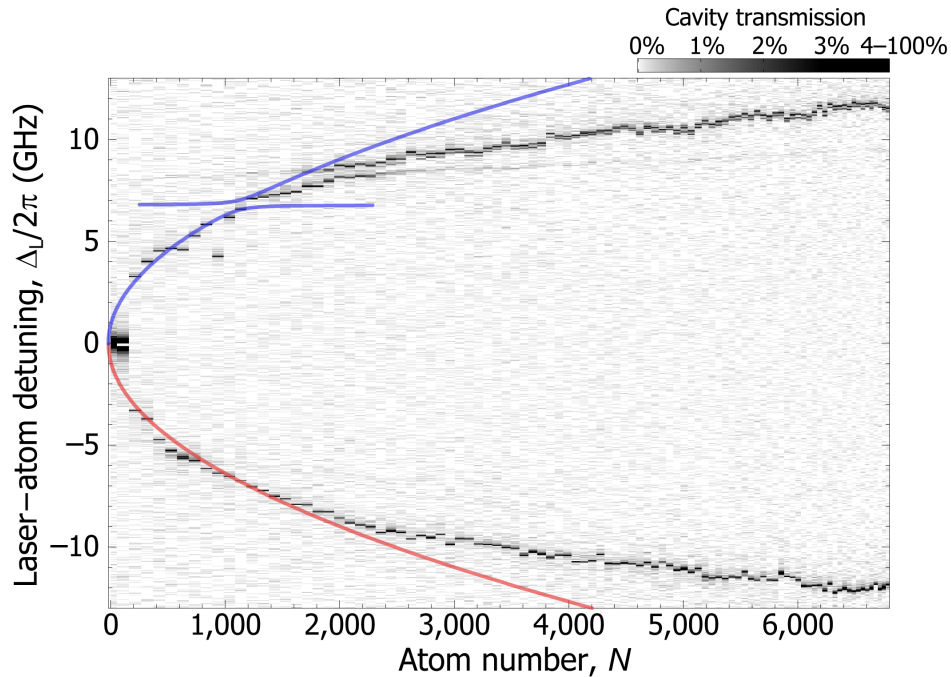
Supplementary figure 2: Eigenenergies computed using the simple multilevel model with $\Delta_{\mathrm{C}} = 0$, $\alpha = 0$, $\beta = 1$, $N_1/N_2 = 0.25\%$, superimposed on the experimental data of Fig. 3a (main text).

$g_1 \sqrt{N_2} = \Delta_{\mathrm{HFS}}$ is fulfilled. It is located at $\delta = \Delta_{\mathrm{HFS}}$ and has a frequency gap $\sim \beta g_1 \sqrt{N_1}$. We adjust the parameters of the model to reproduce the frequency gap $\sim 500\,\mathrm{MHz}$ of the experimental data (Fig. 3a in the main text). Since the polarization of the cavity field is not precisely known, β is unknown and set to 1 for simplicity. The only magnetically trapped state of $5\mathrm{S}_{1/2} |F = 1\rangle$ is $|F = 1, m_F = -1\rangle$, hence we assume that $|F = 1\rangle$ atoms should be this Zeeman substate. As $\alpha \propto \langle \mathrm{g}_2 | \hat{V}_1^2 | \mathrm{g}_1 \rangle$, α is expected to be zero since there is no 2-photon transition between states $|F = 2, m_F = 2\rangle$ and $|F = 1, m_F = -1\rangle$. A finite value for α would lead to additional anticrossings in the spectrum, located at detunings $\delta = \pm \Delta_{\mathrm{HFS}}/2$, which we do not observe in this experiment. The remaining parameter is the $|F = 1\rangle$ population fraction N_1/N_2 — supposed constant regardless of the total number of atoms — which we fit to the data, finding $N_1/N_2 = 0.25\%$. The corresponding resonance curves are shown in Supplementary figure 2. The anticrossing predicted by the model does not occur at the detuning at which it is observed experimentally ($\delta_{\mathrm{exp}} \approx 8.5\,\mathrm{GHz}$). Note also that the asymptotes in the experimental spectrum clearly have nonzero slope, whereas the model predicts horizontal asymptotes. In a more refined model we have taken into account the optical pumping of the atoms arising during the excitation of the coupled system, but found that this effect remains negligible.

An anticrossing related to the hyperfine structure of the ground state is observed by Brennecke *et al.* [S5]. The authors develop a model similar to ours, but including also the complete structure of the D_2 transition, the presence of two light polarizations in the cavity, and a "Lamb-shift" effect due to higher order transverse modes of the cavity. However, as we have checked, none of these effects can account for the position of the anticrossing or the non-zero slope of the asymptotes present in our experimental data. In particular, the first higher order transverse mode of our FFP1 cavity lies some $750\,\mathrm{GHz}$ above the TEM_{00} mode, which is too far detuned to affect the measured spectrum.

Further theoretical and experimental investigations are required to explain the origin and characteristics of the observed anticrossing.

4

3 Heating rate model

In the experiments shown in Fig. 4 (main text), a magnetically trapped BEC interacts with the cavity field for $t_{\mathrm{int}} = 10\,\mathrm{ms}$, with $\Delta_{\mathrm{L}} = \Delta_{\mathrm{C}} = 0$. The heating of the trapped cloud is measured using absorption imaging after a time-of-flight (TOF) expansion $t_{\mathrm{TOF}} = 2.8\,\mathrm{ms}$.

We calculate the heating rate of the trapped cloud with a momentum diffusion model. Fischer *et al.* [S6] derive the diffusion for an untrapped atomic cloud in a cavity in the low saturation limit. In the resonant case ($\Delta_{\mathrm{L}} = \Delta_{\mathrm{C}} = 0$), the momentum diffusion coefficient for the atom i, defined by $\frac{\mathrm{d}}{\mathrm{d}t}(\langle \mathbf{p}_i^2 \rangle - \langle \mathbf{p}_i \rangle^2) \equiv 2D_p^i$, is

$$D_p^i = \frac{n(\hbar k)^2 g_1(\mathbf{r}_i)^2}{\gamma} + \frac{n\hbar^2 (\boldsymbol{\nabla} g_1(\mathbf{r}_i))^2}{\gamma}\,, \tag{11}$$

where n is the intracavity photon number in the presence of the N atoms and $g_1(\mathbf{r}_i)$ is the coupling strength for the atom i, $g_1(\mathbf{r}_i) = g_0 \cos(kx_i) \exp(-r_{\perp i}^2/w^2)$.

The first term in (11) can be rewritten $(\hbar k)^2 \Gamma_{\mathrm{sp}}^i/2$, where Γ_{sp}^i is the rate of spontaneous emission of the atom i. This part of the diffusion process is equivalent to a random walk with step length $\hbar k$, at a rate Γ_{sp}^i, and corresponds to the emission of spontaneous photons in random, isotropically distributed directions. The second term is associated with the randomness of the direction of the absorbed photons. Neglecting the radial contribution in $\boldsymbol{\nabla} g_1$, the two terms have the same average value as soon as the cloud size is large compared to $\lambda/2$. This is the case in the experiments of Fig. 4 (main text), where the calculated diameter of the condensate along the cavity axis is $2R_x = 6.6\,\mu\mathrm{m}$.

Expressing n in terms of the number of photons n_{res} in the empty cavity with the same probe beam intensity, we write the average diffusion as a function of the collective cooperativity C_N:

$$D_p = \frac{2n_{\mathrm{res}}(\hbar k)^2 \kappa}{N} \frac{2C_N}{(1 + 2C_N)^2}\,. \tag{12}$$

The diffusion is maximal for $C_N = 0.5$. Given the small radial extension of the BEC ($2\sigma_{y,z} = 490\,\mathrm{nm} \ll w = 3.9\,\mu\mathrm{m}$), we neglect the variation of the coupling in the transverse directions over the atomic sample: $g_1(x, r_{\perp i}) \equiv g_1(x, r_{\perp})$. This yields a straightforward radial dependence for C_N, $C_N = \frac{1}{2} N C_0 \exp(-2\, r_{\perp}^2/w^2)$ where $C_0 = g_0^2/2\kappa\gamma$ is the maximum single-atom cooperativity. Replacing N, C_0 and w with their values in the experiment, the diffusion peaks are expected to occur when the condensate is positioned about $10\,\mu\mathrm{m}$ off-axis, which is consistent with our measurements.

After the interaction time t_{int}, the probe field is shut off and the atoms are brought to the centre of the mode in $t_{\mathrm{transp}} = 22\,\mathrm{ms}$. This provides identical TOF conditions regardless of the initial radial position $|z_a| \equiv r_{\perp}$ of the cloud, and allows the sample to thermalize. We calculate the cloud r.m.s. sizes $\sigma_{x,y,z}$ after TOF assuming that the energy imparted by the heating is equally redistributed among the 6 degrees of freedom of the trap. This leads to

$$\sigma_x^2 \approx \sigma_{x,\mathrm{ref}}^2 + \frac{1}{3}\frac{D_p\, t_{\mathrm{int}}\, t_{\mathrm{TOF}}^2}{M_{\mathrm{Rb}}^2}\,, \tag{13}$$

and to similar expressions for the y and z directions. M_{Rb} is the $^{87}\mathrm{Rb}$ mass and $\sigma_{x,\mathrm{ref}}$ is the cloud r.m.s. size after TOF when the probe beam is kept off. In (13) we neglect the contribution of the increase in the trapped cloud size, which is a fair approximation. Supplementary figure 3 compares the calculated σ_x with the experimental data; $\sigma_{x,\mathrm{ref}}$ is set to its measured value $\sigma_{x,\mathrm{ref}} \approx 7\,\mu\mathrm{m}$. The calculated diffusion coefficient $D_p^{\mathrm{peak}} = n_{\mathrm{res}}(\hbar k)^2 \kappa/2N$ at the two maxima of heating leads to an almost isotropic cloud after TOF expansion — as is observed experimentally — with $\sigma^{\mathrm{peak}} = v_{\mathrm{rec}}\, t_{\mathrm{TOF}}\, (n_{\mathrm{res}}\, \kappa\, t_{\mathrm{int}}/6N)^{1/2}$, where v_{rec} is the recoil velocity. The numerical value $\sigma^{\mathrm{peak}} = 28\,\mu\mathrm{m}$ overestimates the experimental value $\sigma_{\mathrm{exp}}^{\mathrm{peak}} = 18\,\mu\mathrm{m}$. There are at least two reasonable explanations for that: first, the measured value for the atom number N can be inaccurate up to a factor 2, yielding a factor $\sqrt{2}$ for the cloud final size, consistent with the other experiments which also suggest that the atom number is underestimated; second, as we estimate below, the number of trapped atoms changes during the interaction with the cavity due to optical pumping, thereby changing the value of C_N. This second effect may also explain why the diffusion peaks are broader than expected.
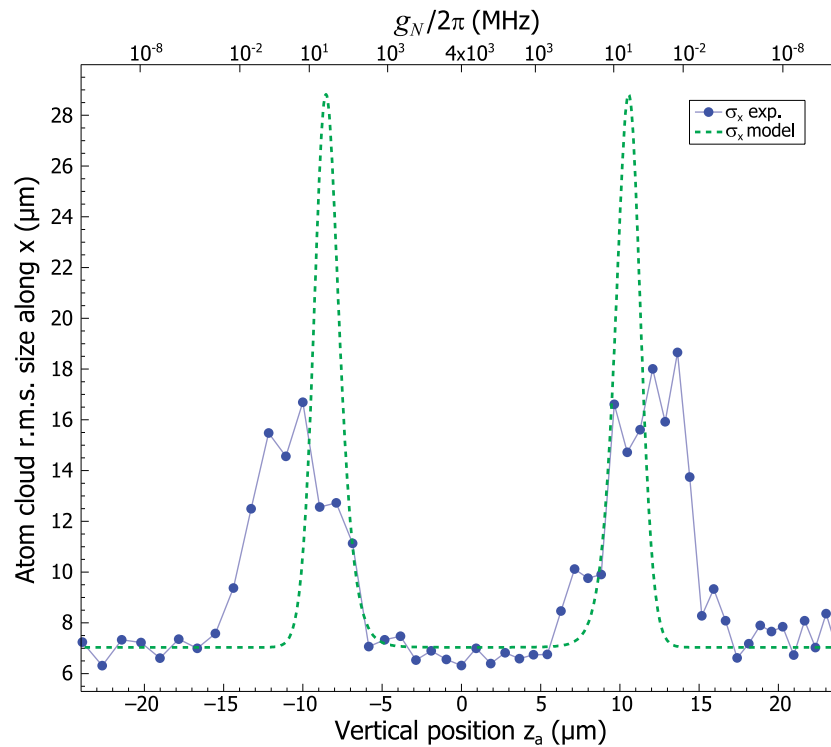
Supplementary figure 3: Calculated r.m.s. cloud size along x after $t_{\mathrm{TOF}} = 2.8\,\mathrm{ms}$, compared to the experimental data shown in Fig. 4 (main text).

The model gives the number of spontaneous emissions per atom at the heating peaks $n_{\mathrm{sp}}^{\mathrm{peak}} = n_{\mathrm{res}}\,\kappa\,t_{\mathrm{int}}/2N \approx 8$, and allows to check the validity of the low-saturation assumption: $P_{\mathrm{exc}}^{\mathrm{peak}} = \Gamma_{\mathrm{sp}}^{\mathrm{peak}}/2\gamma = 2 \times 10^{-5} \ll 1$. Taking the direction x of the magnetic field $\mathbf{B}_0$ at the bottom of the trap as quantization axis, a linear polarization in the cavity is an equal-weight combination of σ^+ and σ^- polarizations. A crude calculation based on branching ratios shows that about 15% of the spontaneous emission events drive the magnetically trapped $|F = 2, m_F = 2\rangle$ atoms into the untrapped states $|F = 1, 2, m_F = 0\rangle$ (free falling) and $|F = 1, m_F = 1\rangle$ (expelled from the trap). This means that a fraction $\gtrsim 0.85^8 = 27\%$ of the atoms stay in the initial state after interaction, in rough agreement with the measurements (the number of detected atoms drops by about 50% at the heating peaks).

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