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Coding Quantum Information in Van Der Waals Repulsive States

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Abstract- Van der Waals interactions are dipole-dipole interactions. In this article, we study the quantum information storage using repulsive van der Waals interaction coupled states. It is shown that if one atom is excited, the second excited atom will be able to change the state distribution of the first excited atom. This can be used to do remote control at the quantum level. In addition, by analyzing the components of the first excited atom, the distance between the two excited atoms and the state distribution of the second excited atom can be extracted. Such systems are essential for developing single-atom quantum sensors.

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Coding Quantum Information in Van Der Waals Repulsive States

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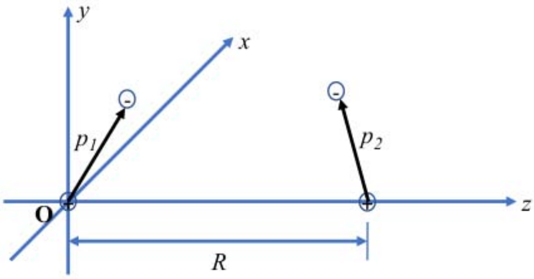

Fig. 1

I. Introduction

Van der Waals interactions are the second-order dipole-dipole interactions, which are proportional to $\frac{1}{R^6}$. Compared to the first-order dipole-dipole interactions, which are proportional to $\frac{1}{R^3}$, van der Waals interactions can be purely repulsive or attractive. Attractive interactions will lead to collisions. On the other hand, repulsive van der Waals interactions will less likely cause collisions. Recent experiments [?] do show that repulsive states lead to a longer coherent time. This offers a variety of opportunities for using repulsive van der Waals interactions for quantum sciences. For example, repulsive van der Waals interactions can be used for quantum gates [? ?]. Here we use electric-dipole electric-dipole interactions as an example. More specifically, we use a Rydberg atom [? ?] as an electric dipole. Therefore, the dipole-dipole interactions are Rydberg atom-Rydberg atom interactions. Such systems are especially useful for developing quantum sensors, especially single-atom sensors.

This paper is arranged in the following way: the theory is presented in the next section, which is followed by discussions about storing and extracting quantum information.

II. Theory

Van der Waals interactions have been studied in the past [? ? ?]. Here we will introduce repulsive van der Waals interactions. We first consider two excited atoms as shown in Fig. **??**, and we apply the Born-Oppenheimer approximation, assuming the ion cores have zero

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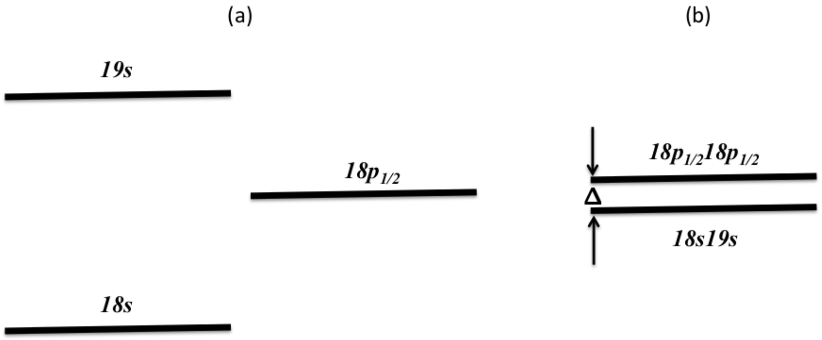

Fig. 2: (a) The atomic energy levels for s and p states. (b) Dimer energy levels, where Δ is the energy difference between the 18s19s and $18\text{p}_{1/2}18\text{p}_{1/2}$.

kinetic energy. We first consider the simplest dipole-dipole interactions between two bodies as shown in Fig. **??**(a). The two-body dipole-dipole interaction potential energy can be expressed as [?]:

$$V_{dd} = -\frac{1}{4\pi\epsilon_0}\frac{p_1p_2(C^1_{1,-1}C^2_{1,1} + C^1_{1,1}C^2_{1,-1} + 2C^1_{1,0}C^2_{1,0})}{R^3}, \tag{1}$$

where $p_1 = er_1$ and $p_2 = er_2$ are the dipole moments of atom 1 and atom 2 respectively. e is one electron charge, and r_1 and r_2 are the radii of atom 1 and atom 2. R is the internuclear spacing between atom 1 and 2. $C_{k,q}$ is the spherical tensor in Edmonds [?], which is a normalized spherical harmonic tensor.

For simplicity, we will focus on the two-body interactions. We use ^{85}Rb as an example. Fig. **??** shows two strongly dipole-dipole coupled states, 18s19s and $18\text{p}_{1/2}18\text{p}_{1/2}$. The energy differnce between those two states is Δ=774.56 MHz as shown in Fig. **??**(b). Here we use frequency to represent energy, since frequency is often used experimentally and the relation between energy E and frequency, f, is $E = hf$, where h is the Planck constant. These two states are calculated by calculating the dimer energies as a function of the principal quantum number n. Fig. **??** shows the energy difference between $\text{np}_{1/2}\text{np}_{1/2}$ and ns(n+1)s, $\Delta{=}E_{np_{1/2}np_{1/2}} - E_{ns(n+1)s}$, as a function of the principal quantum number n. It is shown that at n=18, the absolute energy difference is minimized.

Experimentally, the two-atom excitation can be achieved in a big molecule using the dipole-blockade effect [? ? ? ? ? ? ? ? ? ? ?]. For two-body van der Waals interactions, we consider two energetically close energy levels with energy detuning, Δ. Those

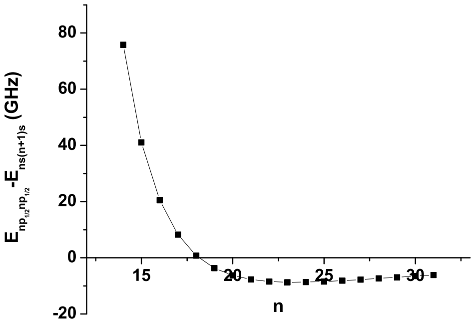

Fig. 3: The energy difference between np $_{1/2}$np$_{1/2}$ and ns(n+1)s as a function of the principal quantum number n.

two levels couple with dipole-dipole interactions, V_{dd} as shown in Eq. **??**. According to the perturbation theory, the eigenenergy and eigenfunctions can be calculated by diagonalizing the following matrix [**?**]:

$$\begin{pmatrix} 0 & < V_{12} > \\ < V_{21} > & \Delta \end{pmatrix}, \tag{2}$$

where

$$< V_{12} > = < \Psi_1^0 | V_{dd} | \Psi_2^0 > = < V_{21} > = V. \tag{3}$$

$\Psi_1^0 = |18s19s>$ and $\Psi_2^0 = |18p_{1/2}18p_{1/2}>$ are the eigen functions of the system without perturbation, or without van der Waals interactions. We further simplify the problem by assuming the left atom is in the 18s state and the right atom is in the 19s state. Δ=774.56 MHz. Diagonalizing the matrix in Eq. (**??**) gives rise to the eigen energies, λ_1 and λ_2,

$$\lambda_{1,2} = \frac{\Delta \pm \Delta\sqrt{1 + \frac{4V^2}{\Delta^2}}}{2}, \tag{4}$$

It can be shown that the eigen energies are proportional to $\frac{1}{R^6}$, if $V << \Delta$. This is the well known R^{-6} dependence for van der Waals interactions [**?**].

The normalized eigen functions are Φ_1 and Φ_2:

$$\Phi_1 = \frac{2V}{\sqrt{8V^2 + 2\Delta^2 + 2\Delta\sqrt{\Delta^2 + 4V^2}}}\Psi_1^0 + \frac{\Delta + \sqrt{\Delta^2 + 4V^2}}{\sqrt{8V^2 + 2\Delta^2 + 2\Delta\sqrt{\Delta^2 + 4V^2}}}\Psi_2^0, \tag{5}$$

and

$$\Phi_2 = \frac{2V}{\sqrt{8V^2 + 2\Delta^2 - 2\Delta\sqrt{\Delta^2 + 4V^2}}}\Psi_1^0 + \frac{\Delta - \sqrt{\Delta^2 + 4V^2}}{\sqrt{8V^2 + 2\Delta^2 - 2\Delta\sqrt{\Delta^2 + 4V^2}}}\Psi_2^0. \tag{6}$$

Ψ_1^0 and Ψ_2^0 are the eigen functions of the system without the perturbation V. From the wave functions, it is shown that the wavefunctions depend on V, and V depends on the internuclear spacing R, V$\propto \frac{1}{R^3}$. Therefore, the components of the wave functions will change as a function of the internuclear spacing.

For example, we first excite one atom, the left atom, to an 18s state. This state will be a pure 18s state. We then excite a second atom, the right atom, to a 19s state. By the time, the second atom is excited, the first atom, or the left atom, is no longer a pure 18s state, it will have the 18p$_{1/2}$ component caused by the van der Waals interactions between the two excited atoms. Therefore, the component change caused by the excitation of the second atom can be used for remote control, since the two atoms are separated. In addition, by analyzing the left atom, or checking the amount of the s component and p component, the distance between those two excited atoms can be calculated. In addition, depending on the component of the first atom, the components of the second atom can be calculated.

The plot for the energy levels and the probabilities of the wavefunctions are shown in Figs. **??** and **??**. Fig. **??** shows that the 18s19s state is an attractive state, and 18p$_{1/2}$18p$_{1/2}$ is a repulsive state. Let's focus on the 18s19s state. Again, we consider that the left atom is excited to the 18s state first, and the right atom is then excited to the 19s state. Depending upon the distance between those two atoms, once the 19s atom is excited, the 18s atoms will change components. For example, if the distance between those two atoms is about 0.2 μm, once the 19s atom is excited, about 40% of the left atom, the 18s atom, will change to 18p$_{1/2}$ as shown in Fig. **??**(b). Such interaction, without direct contact, can be used for remote control. From Fig. **??**(b), it is shown that the probability of 18s19s state is 1 at R$\to\infty$. As the internuclear spacing decreases, the amount of 18p$_{1/2}$18p$_{1/2}$ increases, and the amount of 18s19s decreases. In addition, the probabilities depend on the internuclear spacing R. Therefore, by detecting the amount of 19s atom in the right atom, the internuclear spacing can be extracted. In addition, by knowing the amount of 19s sate, the amount of 18p$_{1/2}$ in both atoms and the amount of 18s atom can be extracted.

In previous sections, we excite the left atom to 18s and the right atom to 19s. It is more interesting to investigate if we excite both atoms to 18p$_{1/2}$ states, which is a purely repulsive state, the red solid line as shown in Fig. **??**. The repulsive states are especially useful for practical applications, such as quantum gates. Compared to attractive states, repulsive states are less likely to cause collisions, and those states have longer coherent

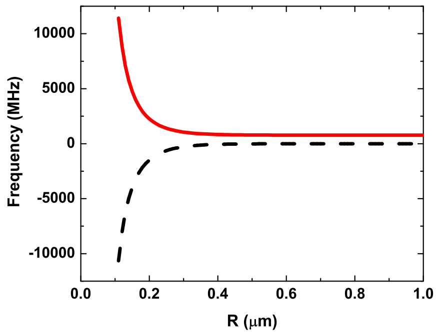

Fig. 4: The energy level 18s19s (black dash line − − −) and $18p_{1/2}18p_{1/2}$ (red solid line ——) as a function of the principal quantum number n.

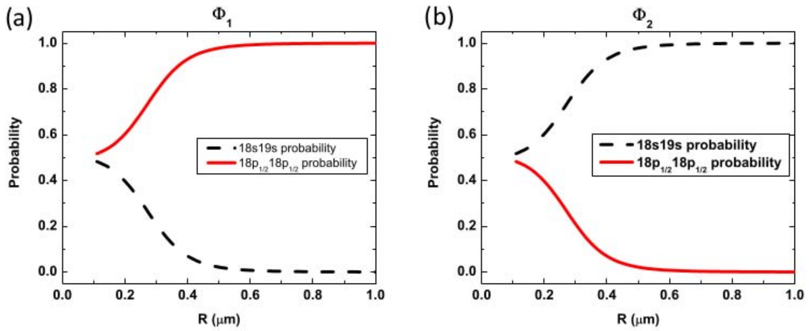

Fig. 5: (a) The probability of 18s19s (black dash line − − −) and $18p_{1/2}18p_{1/2}$ (red solid line ——) in Φ_1 as shown in Eq. (**??**). (b) The probability of 18s19s (black dash line − − −) and $18p_{1/2}18p_{1/2}$ (red solid line ——) in Φ_2 as shown in Eq. (**??**).

times [**?**]. For example, if we first excite the left atom to the $18p_{1/2}$ state and then excite the right atom to $18p_{1/2}$ state, how would the first excited atom, or the left atom, change? Would one part of the atom change to 18s state, 19s state, or both? This is a quantum mechanics problem. Here we consider the matrix composed by the following three states: $\Psi_1'^0 = |18s19s>$, $\Psi_2'^0 = |19s18s>$, and $\Psi_3'^0 = |18p_{1/2}18p_{1/2}>$ by considering the exchange symmetry. To show that this case is different from the previous case, we add prime in the labels for eigenenergies and eigenfunctions. The Hamiltonian can then be written as

$$\begin{pmatrix} 0 & 0 & V \\ 0 & 0 & V \\ V & V & \Delta \end{pmatrix}, \tag{7}$$

where V is the matrix element shown in Eq. (**??**). The eigen energies are

$$\lambda_1' = 0, \tag{8}$$

$$\lambda_2' = \frac{\Delta - \Delta\sqrt{1 + \frac{8V^2}{\Delta^2}}}{2}, \tag{9}$$

$$\lambda'_3 = \frac{\Delta + \Delta\sqrt{1 + \frac{8V^2}{\Delta^2}}}{2}. \tag{10}$$

The eigen functions are

$$\Phi'_1 = \frac{1}{\sqrt{2}}(-\Psi'^{0}_{1} + \Psi'^{0}_{2}), \tag{11}$$

$$\Phi'_2 = \frac{1}{\sqrt{8V^2 + \Delta^2 - \Delta\sqrt{\Delta^2 + 8V^2}}}[\sqrt{2}V\Psi'^{0}_{1} + \sqrt{2}V\Psi'^{0}_{2} + (\frac{\Delta - \sqrt{\Delta^2 + 8V^2}}{\sqrt{2}})\Psi'^{0}_{3}], \tag{12}$$

$$\Phi'_3 = \frac{1}{\sqrt{8V^2 + \Delta^2 + \Delta\sqrt{\Delta^2 + 8V^2}}}[\sqrt{2}V\Psi'^{0}_{1} + \sqrt{2}V\Psi'^{0}_{2} + (\frac{\Delta + \sqrt{\Delta^2 + 8V^2}}{\sqrt{2}})\Psi'^{0}_{3}], \tag{13}$$

where Ψ'^{0}_{1}, Ψ'^{0}_{2}, and Ψ'^{0}_{3} are the eigen functions of the system without the perturbation V. If the left atom is excited to the $18\mathrm{p}_{1/2}$, the right atom is then subsequently excited to the same state. Due to the strong coupling between the $18\mathrm{p}_{1/2}18\mathrm{p}_{1/2}$, 18s19s, and 19s18s, 18s and 19s atomic states will be mixed in the $18\mathrm{p}_{1/2}18\mathrm{p}_{1/2}$ state. From Eqs.12 and 13, it is shown that Ψ'^{0}_{1}=18s19s and Ψ'^{0}_{2}=19s18s have an equal amount of probability. In other words, if the left atom is excited to the $18\mathrm{p}_{1/2}$, the right atom is then excited to the $18\mathrm{p}_{1/2}$, the components of each $18\mathrm{p}_{1/2}$ atom will change to a mixture of three states $18\mathrm{p}_{1/2}$, 18s, and 19s. That is, the probability of having 18s is the same as the probability of having 19s.

Adding more atoms in the system will lead to the complexity of the system. On the other hand, more information will be stored in such systems. The primary challenge is how to individually address each state of the system, which requires precision measurement.

III. Conclusion

In conclusion, we have shown a step to step evaluation for using van der Waals coupled states to store quantum information. More specifically, we discussed a two-atom system. It is shown that by analyzing the components of one atom, the distance between those two atoms can be extracted, and the components of the other atom can be predicted. This can be used for remote control. Furthermore, one pair of repulsive states lead to more interesting results that originated from quantum mechanics.

Acknowledgement

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