

# Coherence conditions for groups of Rydberg atoms

**J V Hernández and F Robicheaux**

Department of Physics, Auburn University, AL 36849-5311, USA

E-mail: [hernajv@physics.auburn.edu](mailto:hernajv@physics.auburn.edu)

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## Abstract

We investigate the excitation of a collection of cold atoms to Rydberg states. By a direct numerical solution of Schrödinger's equation, we are able to compute various interesting properties of the many-body wavefunction. The high polarizability of Rydberg atoms allows them to support large dipole moments which in turn can interact with each other over long ranges. If the interaction energy between excited atoms is large enough, the resultant energy shift will move the two excitation states out of resonance, thus effectively blocking a two excitation state from occurring. One particular topic investigated is the quantum phase gate, where both groups of atoms are within a blockade radius  $R_b$  and subjected to a  $\pi - 2\pi - \pi$  sequence of pulses. We examine the regime where the groups are neither totally within nor totally outside the blockade radius. Our results explore the tolerance in variation of intergroup lattice distances for a series of quantum gates.

## 1. Introduction

Atoms excited into Rydberg states are large in size and thus able to support large dipole moments. The long-range interactions between these large dipoles have been a popular topic of study over the last several years. With recent advancements in cooling and trapping, it has been experimentally shown that the laser excitation of a frozen gas from an initial state to a Rydberg state is suppressed when driving on resonance [1–5]. There have also been various numerical simulations investigating this system [1, 6–8]. If the interaction energy between two excited atoms is large enough, the shift will move the two excitation state out of resonance, thus effectively blocking this state from occurring. The number of particles able to be excited is now suppressed, exhibiting a dipole blockade [9]. This allows for the coherent manipulation of a large collection of atoms, enabling careful macroscopic control over microscopic systems. The ability to precisely interact with quantum systems is critical in the development of quantum computing.

The original proposals for creating a dipole blockade [10] consisted of exciting Rydberg states at Förster resonance and using the interaction between these transition dipole moments to create energy shifts. Evidence of a dipole blockade has been successfully observed via this

process [2]. A dipole blockade could also be created by exciting a group of cold Rydberg atoms in a static electric field (*along the z-axis*). The resultant Stark states have relatively large static dipole moments,  $\vec{d}$ , along the direction of the electric field. For two Rydberg atoms within the  $n$  manifold in a static electric field, separated by a distance  $R$ , the dominant long-range interaction is proportional to  $1/R^3$  and scales like  $n^4$ . This is similar to the proposal for a blockade that utilizes the second-order interaction (van der Waals) between two np Rydberg atoms [1]. It is proportional to  $1/R^6$  and scales like  $n^{11}$ . In this paper we will investigate both the first-order dipole–dipole and second-order van der Waals (vdW) interactions. For the vdW case, we will only be looking at the ns–ns interaction in order to eliminate any directional dependence. In both cases, the initial state is coherent; we do not include decays or repopulations from our ‘ground’ level. If a narrow bandwidth laser is used to drive from the ‘ground’ to a high Rydberg state ( $n > 50$ ) on resonance, the main transition will be the dipole-allowed one [11]. We can then treat the entire collection as a group of two-level systems.

When a collection of cold atoms is in a blockade configuration (i.e. the physical parameters are such that the interaction energy between two Rydberg atoms is large enough to shift the pair out of the two excitation resonance), the number of atoms that can be excited ( $N_e$ ) is suppressed. By taking repeated measurements of  $N_e$ , we can find the relationship between the mean  $\langle N_e \rangle$  and the variance  $\langle N_e^2 \rangle - \langle N_e \rangle^2$ . The Mandel  $Q$  parameter,  $Q \equiv \frac{\langle N_e^2 \rangle - \langle N_e \rangle^2}{\langle N_e \rangle} - 1$ , is a useful quantity to compare the atom counting statistics to a Poissonian distribution [12]. For a Poissonian distribution the mean is equal to the variance, so  $Q = 0$ . In the case of blocked atoms,  $Q$  should be less than 0; this corresponds to a sub-Poissonian distribution. The  $Q$  parameter reflects the measure of how efficiently the system is blocked. Recent experiments have been able to measure  $Q$  values [4] and in this paper we will present the results of our simulations of  $Q$ .

We also investigate the situation where there are two spherical, localized groups of cold atoms. The radii of both spheres are chosen so that all pairs of atoms are in a blockade configuration when the two spheres are just touching. The maximum number of atoms able to be excited in this case should be 1, creating a two-level system. We then subject the system to the following sequence of pulses: group 1 is excited by a  $\pi$  pulse, then group 2 is excited by a  $2\pi$  pulse and finally group 1 is deexcited by another  $\pi$  pulse. If all pairs of atoms are in a blockade configuration, the sequence of pulses will maintain all the atoms in their ‘ground’ level, but this final state will now have a  $\pi$  phase shift relative to the initial state. This sequence of pulses acts as a phase gate [9]. If the radii of each sphere are held constant and the centre-to-centre distance  $D$  is increased, pairs of intergroup atoms will no longer be blocked. There is no longer just a two-level system, but if  $D$  is increased to the point where no intergroup atoms are blocked, then each group is now effectively independent of the other leaving two two-level systems. In such a configuration, the  $\pi - 2\pi - \pi$  pulse will leave the final state exactly in phase with the initial one. Our interest is in the regime in between all intergroup atoms being blocked and none of them being so. The behaviour of the phase gate as  $D$  is increased will determine how far apart or close together the groups of atoms must be in order to minimize errors.

The relatively large and long-range interaction between a pair of Rydberg atoms implies that a collection of  $N$  atoms must be treated as a many-body system. By a direct numerical solution of Schrödinger’s equation, we are able to compute and retain various interesting properties of the many-body wavefunction. Even if every atom was strictly treated as a two-level system, the number of basis states needed for a direct solution would still be  $2^N$ . This severe limitation in size can be overcome by utilizing the simplifications described in [7].

Although the method used in this paper utilizes the full wavefunction for calculations, other techniques have been used such as the Monte Carlo procedure used in [6] which requires much less computational effort. This is appropriate in the case of an incoherent ground state such as in [4], but it cannot be used to probe quantities such as phase shifts or the amplitudes of pieces of the full wavefunction useful to quantum computing. The mean field approach developed in [1] works well for high laser power, but it is unable to give spatial correlation functions or phase shifts needed to check the error of phase gates. Unless otherwise noted, atomic units will be used throughout this paper.

## 2. Theory

In this section we will describe the techniques involved in the direct numerical solution to the many-atom wavefunction. We will also discuss how we solved for the wavefunction in a manner that allowed us to check for convergence. Once the wavefunction has been solved for, it is possible to compute the number of excited atoms and various correlation functions.

We begin by treating each atom as a purely two-level system with one level being the initial tightly bound state  $|g\rangle$  and the other being a highly excited Rydberg state  $|e\rangle$ . For the purposes of this paper, the locations of the atoms will be fixed in space. This is a reasonable approximation if the temperature of the gas is low enough and the time duration of the exciting laser pulse is short enough. For conditions similar to recent experiments, the laser pulse must be  $\lesssim 200$  ns. We expanded the wavefunction

$$|\Psi(t)\rangle = a_{gg\dots g}(t)|gg\dots g\rangle + a_{eg\dots g}(t)|eg\dots g\rangle \\ \dots + a_{ee\dots g}(t)|ee\dots g\rangle + a_{ee\dots e}(t)|ee\dots e\rangle \quad (1)$$

$$= \sum_{\alpha} a_{\alpha}(t)|\alpha\rangle. \quad (2)$$

We do not use all of the states in the expansion, but recursively eliminate them as described in [7]. At time  $t = 0$ , all atoms are in their tightly bound state:  $|\Psi(0)\rangle = |gg\dots g\rangle$ .

The Hamiltonian of this system is

$$\hat{H} = \sum_j \hat{H}_j^{(1)} + \sum_{j < k} V_{jk} |e_j e_k\rangle \langle e_j e_k|, \quad (3)$$

$$\hat{H}_j^{(1)} = -\Delta\omega(t) |e_j\rangle \langle e_j| + \frac{\mathcal{S}}{\tau} e^{-t^2/\tau^2} (|g_j\rangle \langle e_j| + |e_j\rangle \langle g_j|),$$

where  $V_{jk}$  is the interaction between two excited states for an atomic pair  $(j, k)$ . The detuning of the laser is  $\Delta\omega(t)$ ,  $\tau$  is proportional to the duration of the excitation pulse, and  $\mathcal{S}$  is the laser amplitude. The Hamiltonian was also obtained by using the rotating wave approximation. If we use parameters similar to [1], the laser frequency is in the UV range and at a relatively low intensity, allowing for the rotating wave approximation to be a good one. If, however, the parameters in [5] are used and a microwave transfer pulse is introduced, then careful consideration must be used when applying this approximation. If the detuning is set to zero and the system is blockaded, the system evolves in an oscillatory manner between all the atoms in the ground state and a symmetrical state with only one excited Rydberg atom. The Rabi frequency is  $\sqrt{N}\Omega$ , where  $\Omega$  is the single atom Rabi frequency and  $N$  is the number of atoms blocked. The dynamics of this two-level system can be given as

$$\begin{bmatrix} a_g(t) \\ a_e(t) \end{bmatrix} = \begin{bmatrix} \cos \theta(t) & -i \sin \theta(t) \\ -i \sin \theta(t) & \cos \theta(t) \end{bmatrix} \begin{bmatrix} a_g(0) \\ a_e(0) \end{bmatrix}, \quad (4)$$

where  $\theta(t) = 2\sqrt{N} \int_{-\infty}^t (S/\tau) \exp(-t'^2/\tau^2) dt'$ . The probability that one atom will be excited at the end of the laser pulse is  $\sin^2(\sqrt{N\pi}S)$ .

In order to solve Schrödinger's equation numerically, we use the split operator method:

$$|\Psi(t + \delta t)\rangle = e^{-i\hat{H}_{\text{off}}(t)\delta t/2} e^{-i\hat{H}_{\text{diag}}\delta t} e^{-i\hat{H}_{\text{off}}(t)\delta t/2} |\Psi(t)\rangle, \quad (5)$$

where  $\hat{H}_{\text{diag}}$  is the matrix of diagonal elements (Rydberg–Rydberg interaction) of  $\hat{H}$  and  $\hat{H}_{\text{off}}$  is the matrix of off-diagonal elements (laser interaction) of  $\hat{H}$ , such that  $\hat{H} = \hat{H}_{\text{diag}} + \hat{H}_{\text{off}}$ . At this point, the laser part of the interaction is approximated via the second-order Runge–Kutta method. The error introduced is  $O(\delta t^3)$ , but by using second-order Runge–Kutta the norm  $\langle \Psi(t) | \Psi(t) \rangle$  is no longer conserved. In fact at every time step it endures a error  $O(\delta t^4)$ . By using small enough time steps, we are able to minimize this error.

For a group of cold Rydberg atoms in an electric field  $\mathcal{E}$ , the dipole–dipole interaction between atoms  $j$  and  $k$  can be given as

$$V_{jk} = \frac{\vec{d}_j \cdot \vec{d}_k - 3(\vec{d}_j \cdot \hat{R}_{jk})(\vec{d}_k \cdot \hat{R}_{jk})}{R_{jk}^3}, \quad (6)$$

where  $\vec{d}_j$  is the dipole matrix element for atom  $j$ . If the electric field is in the  $\hat{z}$ -direction and we excite to the highest energy Stark state, then the dipole matrix elements can be written as  $\vec{d} = (3/2)n^2\hat{z}$ . Finally, we can write

$$V_{jk} = \frac{9n^4}{4} \frac{1 - 3\cos^2(\theta_{jk})}{R_{jk}^3}, \quad (7)$$

where  $\theta_{jk}$  is the angle formed between the vector pointing from atoms  $j$  to  $k$  and the direction of the electric field. With no electric field, a second-order interaction between two atoms in states  $\nu_0$  and  $\mu_0$ , respectively, takes place:

$$V_{jk} = \frac{1}{R_{jk}^6} \sum_{\nu,\mu} \frac{|\langle \nu | \langle \mu | \vec{r}_j \cdot \vec{r}_k - 3(\vec{r}_j \cdot \hat{R}_{jk})(\vec{r}_k \cdot \hat{R}_{jk}) | \nu_0 \rangle | \mu_0 \rangle|^2}{E_\nu + E_\mu - (E_{\nu_0} + E_{\mu_0})}. \quad (8)$$

This can be more concisely written as  $V_{jk} = -C_6/R_{jk}^6$ , and the  $C_6$  coefficient is proportional to  $n^{11}$ . A major difference between the dipole–dipole and vdW interactions is the dependence on the relative orientation between atoms.

After propagating the wave equation for a period of time, we can now easily determine the fraction of atoms in the excited state by projecting onto the states  $|\alpha\rangle$ :

$$P_e = \sum_{\alpha} \frac{N_{\alpha}}{N} |\langle \alpha | \Psi \rangle|^2 = \sum_{\alpha} \frac{N_{\alpha}}{N} |a_{\alpha}(\infty)|^2, \quad (9)$$

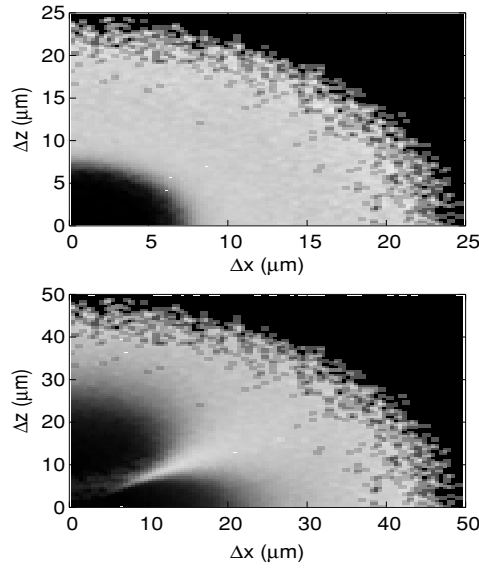
where  $N_{\alpha}$  is the number of atoms excited in state  $|\alpha\rangle$ . It is also possible to calculate a spacial correlation function, which is the probability of finding two excited atoms separated by a distance  $R$  divided by the probabilities of each individual atom:

$$C(R) = \frac{P_{ee}(R)}{P(R)P_e^2}, \quad (10)$$

where  $P_{ee}(R)$  is the probability to find two atoms excited a distance  $R$  apart:

$$P_{ee}(R) = \sum_{j < k} |\langle \beta_{jk} | \Psi \rangle|^2, \quad (11)$$

such that the state  $|\beta_{jk}\rangle$  has excited atoms  $j$  and  $k$  a distance  $R$  apart.  $P(R)$  is the probability of finding a pair of atoms separated by a distance  $R$ . By examining this two-particle correlation function, we can estimate  $R_b$ , the blockade radius [7].



**Figure 1.** The two-particle correlation function for a group of Rydberg atoms. The top graph is for the second-order (van Der Waals) interaction and the bottom graph is for the first-order interaction. The axes are the distances between particles in the  $x$  and  $z$  directions. The grey scale indicates the probability of finding a second Rydberg atom at a location with respect to a Rydberg atom at the origin. Black is the smallest probability. The correlation function drops to zero outside of  $25 \mu\text{m}$  in the vdW case and outside of  $50 \mu\text{m}$ . This is due to the fact that there are no pairs that exist with distances greater than  $2R_0$ , where  $R_0$  is the size of the uniformly distributed sphere.

### 3. Pair correlation

If we take advantage of the azimuthal symmetry of the Hamiltonian and take a slice in the  $xz$  plane, we can look at the 2D pair correlation function. For this simulation, we used ten  $^{85}\text{Rb}$  atoms and randomly placed them using a uniform spatial distribution in a sphere of radius  $R_0$ . For the vdW case,  $R_0 = 12.5 \mu\text{m}$  and for the dipole–dipole case,  $R_0 = 25 \mu\text{m}$ . In both cases, we excite via a  $\pi$  pulse for 120 ns. The top plot in figure 1 is the pair correlation  $C(\Delta x, \Delta z)$  for the vdW interaction. As expected, the vdW case is also symmetric in the polar direction. A reasonably accurate blockade region can be defined by  $R_b$ . If an atom is excited, then all of the other atoms within a distance  $R_b$  are blocked. In the dipole–dipole case (static electric field in the  $\hat{z}$ -direction), the interaction potential depends on  $\theta_{jk}$ , the angle between the electric field and the vector connecting atoms  $j$  and  $k$ . In fact when  $\cos(\theta_{jk}) = \pm\sqrt{1/3}$ ,  $V_{jk} = 0$ ; the interaction vanishes and the two atoms are independent of each other. This can be seen in the bottom plot of figure 1: along the angle  $\cos(\theta_{jk}) = \sqrt{1/3}$  ( $\theta_{jk} \approx 55^\circ$ ), the blockade region is pierced. In order to have a well-defined  $R_b$  as in the vdW case, the geometry must be set up where  $\cos(\theta_{jk}) \neq \pm\sqrt{1/3}$  for as many  $j, k$  pairs as possible. This can be accomplished by placing the atoms in a thin plate in the  $xy$  plane; by decreasing the thickness, we can adjust the number of pairs that lie along the critical angle. If the atoms lie in the  $xy$  plane, then  $C$  is only a function of  $R$ ,  $C \simeq C(R)$ .

The value of  $R_b$  can be estimated by finding at which distance  $V_{jk} \approx \hbar/\tau$ . Since the correlation function is not a perfect step function [7], the value of  $R_b$  is not exact unless a well-defined criterion is set up. In this paper, the blockade radius for a given  $\tau$  is defined as follows: the diameter of the sphere with the largest radius where the maximum number of

atoms that can be excited averages to 1.01. As a test of this definition of  $R_b$ , we computed the probability of being in the blockade state,  $(|egg \dots g\rangle + |geg \dots g\rangle + \dots + |ggg \dots e\rangle)/\sqrt{N}$ , and the phase of the amplitude of the blockade state. When  $\langle N_e \rangle = 1.01$ , then the probability of being in the blockade state is approximately 98% and the phase shift is about  $0.52\pi$ ; for a perfect blockade, these should be 100% and  $\pi/2$ , respectively.

#### 4. Number correlation

The Mandel  $Q$  parameter is a measure of the blockade effectiveness. By solving the many-body wavefunction,  $Q$  is readily found. A value of  $Q = 0$  indicates a perfectly Poissonian distribution. For a collection of  $N$  completely independent, quantum atoms with a probability  $P_e$  of being excited,

$$\langle N_e \rangle = \sum_{j=0}^N \binom{N}{j} j P_e^j (1 - P_e)^{N-j} = N P_e \quad (12)$$

and

$$\langle N_e^2 \rangle = \sum_{j=0}^N \binom{N}{j} j^2 P_e^j (1 - P_e)^{N-j} \quad (13)$$

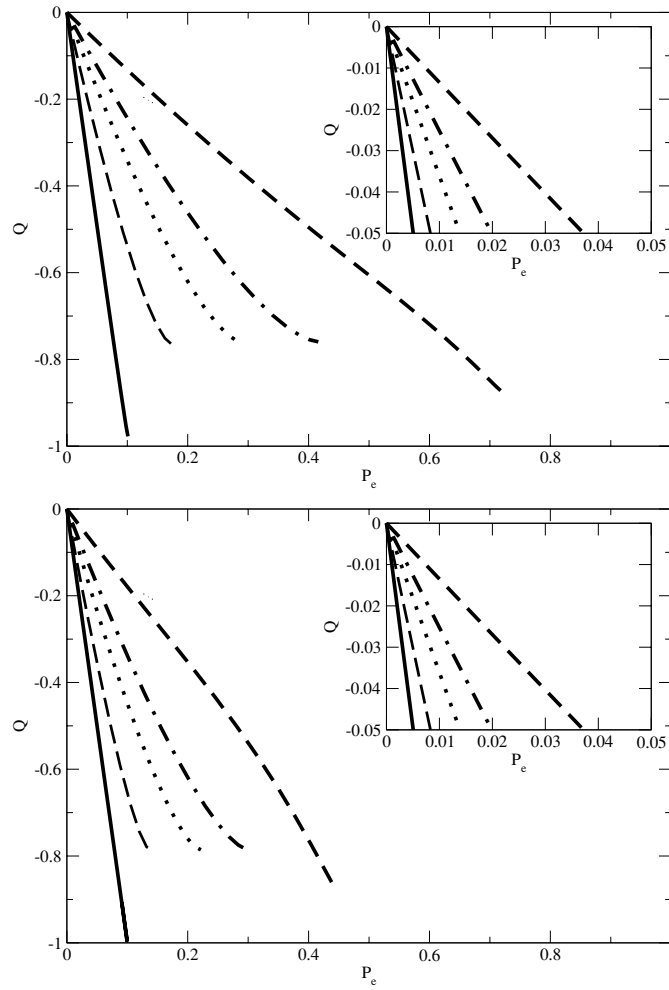
$$= (N P_e)^2 + N P_e (1 - P_e). \quad (14)$$

So for the uncorrelated case,  $Q = -P_e$  (i.e. uncorrelated quantum systems do not give  $Q = 0$ , but minus the fraction excited). The other extreme case is if  $N_b$  atoms are located within a blockade region. Now only up to one atom can be excited; thus,

$$\langle N_e \rangle = N_b P_e \quad (15)$$

$$\langle N_e^2 \rangle = N_b P_e. \quad (16)$$

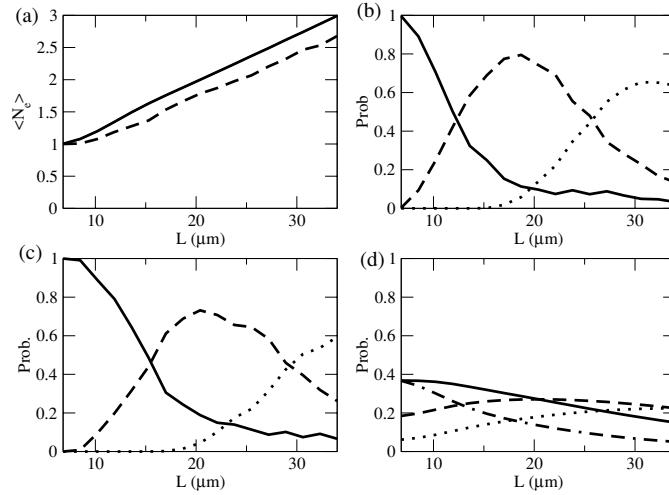
So  $Q = -N_b P_e$  for the case of  $N_b$  atoms being within the blockade radius. In figure 2, the  $Q$  value is plotted as a function of the fraction of atoms excited for different densities:  $\rho_0 \approx 1.3 \times 10^{10} \text{ cm}^{-3}$ ,  $\rho_0/8$ ,  $\rho_0/27$ ,  $\rho_0/64$  and  $\rho_0/512$ . In all cases, ten atoms were used in the simulation. Figure 2(a) was generated using the vdW ( $1/R^6$ ) interaction, while figure 2(b) used the dipole–dipole interaction ( $1/R^3$ ). At the lowest density,  $Q(P_e) \simeq -1P_e$ , indicating a very low level of correlation. In essence, we have a group of isolated two-level systems. As the density is increased, the slope of  $Q(P_e)$  steepens suggesting that the system is becoming more and more highly correlated. Because the dipole–dipole interaction has a longer range than the vdW case, the slope of  $Q(P_e)$  is steeper for the former. The inset examines the system at low laser intensities, or equivalently when few atoms are excited. It can be seen that the slope remains relatively constant in both the vdW and dipole–dipole cases, showing that the system is still correlated even when few particles are excited. Although the excited atoms are not in a blockade configuration with each other, the blocked atoms near by certainly are. These blocked atoms are still ‘conveying’ the information about the system to the separated excited atoms. They are not excited because they are blocked and not just because few atoms are excited. It is the initial state of the system which holds the information, even before the interactions are turned on. By comparing the slope,  $m$ , of  $Q(P_e)$  to the perfectly blocked case, we can in effect measure how ‘efficient’ the interaction is by turning the system from a large collection of uncorrelated two-level systems to a single two-level system. In fact,  $-N/m$  gives a rough indication of how many uncorrelated two-level systems the collection has been reduced to.



**Figure 2.**  $Q$  values as a function of the fraction excited ( $P_e$ ) for different densities. The solid line was calculated using a density  $\rho_0 \approx 1.3 \times 10^{10} \text{ cm}^{-3}$ . Moving from left to right, the densities decrease as follows:  $\rho_0/8$  (dashed),  $\rho_0/27$  (dotted),  $\rho_0/64$  (dash-dotted) and  $\rho_0/512$  (thick-dashed). The inset is a blow-up of the region where there are very few excitations. (a) is for the vdW case and (b) is for the dipole-dipole interaction. The line  $Q = -P_e$  results when the atoms are uncorrelated.

## 5. Filling factor for excitations

If a group of atoms is all within  $R_b$ , then at most only one excitation is allowed. If every excited atom creates a ‘bubble’ of radius  $R_b$  around itself, then in a given volume the maximum number of excited atoms should be approximately the number of bubbles that can fit into that volume. We examined how the maximum number of allowed excitations increases as the volume containing the atoms is increased, while maintaining a fixed density. We focused on the case of the atoms placed in a line because that situation should show the largest effect. We initially placed five atoms on a linear lattice  $1.7 \mu\text{m}$  apart and excited the system to the maximum number excited via a pulse 120 ns long. For these parameters,  $R_b \sim 8.2 \mu\text{m}$ . We then increased the number of atoms in the line and again excited to the maximum  $N_e$ . If the



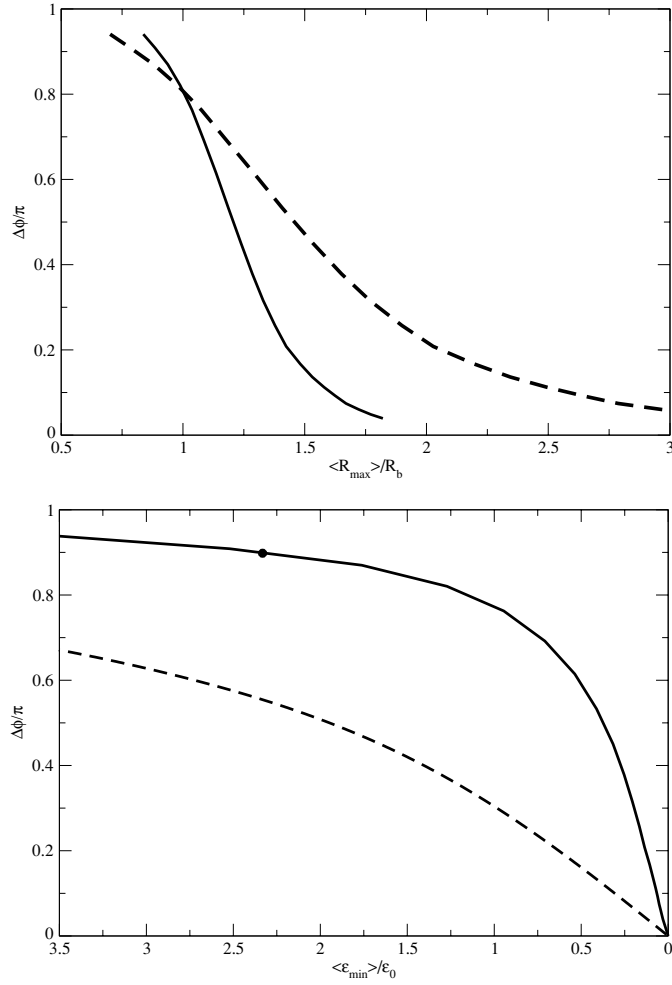
**Figure 3.** (a) is the maximum  $\langle N_e \rangle$  for atoms in a line of length  $L$ . The solid line is for the perfect lattice case while the dashed line is when the atoms are randomly distributed on the line. In (b) the solid line is the probability of being in a state with exactly one atom excited as a function of the length  $L$  for the perfect lattice case. The dashed line is the probability of being in a state with only two atoms excited and the dotted line is the probability of being in a state with three atoms excited, all for the perfect lattice case. (c) is the same plot as 3(b) except for the randomly distributed geometry. (d) is also the same plot as 3(c) and 3(b) except using a Poissonian distribution. The dash-dot line is the probability of zero atoms being excited, the solid is for one excited, the dashed is for two excited and the dotted is for three excited.

‘bubble’ picture is correct, then the maximum number of excited atoms should remain about 1 until two bubbles of radius  $R_b$  can fit into the line then it should jump to 2. We also looked at the non-lattice case where we randomly placed the appropriate number of atoms in the lengths used in the perfect lattice case. In figure 3(a), we plotted the maximum  $\langle N_e \rangle$  as a function of the chain length  $L$ , for both the perfect lattice case and the random case. In either case, the average number of excited atoms rises fairly linearly with the chain length; as soon as there is ‘room’ for more than one excitation  $\langle N_e \rangle$  does not jump up to the next integer number excited.  $\langle N_e \rangle$  fills the region rather smoothly, so the ‘bubble’ picture is not entirely correct. Figures 3(b) and (c) illustrate how states with excited atoms become available as  $L$  is increased. The solid line is the probability of being in a state with only one atom excited, the dashed line is for being in a state with only two excited and the dotted line is for three. The smoothness of figure 3(a) can be accounted for by looking at the probabilities of being in various excited states. By the time the probability of being in a state with only one excited atom is down to around 50%, the probability of being in a state with two excited atoms has risen to about 50%. Figure 3(d) is similar to figures 3(b) and (c) except what is plotted is the probabilities of being in certain states given a Poissonian distribution. As expected, it is quite different from the sub-Poissonian distribution of our correlated system.

## 6. Phase gates

If the system is sufficiently sparse, all the Rydberg atoms act as isolated two-level systems, or, in the parlance of quantum computing, each atom represents an independent qubit. When a group of atoms are all perfectly blockaded, they also form a single two-level system. This group of atoms appears as a two-level system, but it is actually a collection of atoms so tightly





**Figure 4.** Two regions of equal size and density are excited by a  $\pi - 2\pi - \pi$  sequence of pulses in the following manner: group 1 is excited by a  $\pi$  pulse, then group 2 is excited by a  $2\pi$  pulse and finally group 1 is deexcited by another  $\pi$  pulse. (a) shows the phase shift  $\Delta\phi/\pi$  as a function of the average maximum intergroup pair distance,  $\langle R_{\max} \rangle$ , divided by the blockade distance  $R_b$ . The solid line is for the vdW case ( $1/R^6$ ), while the dashed line is for the dipole-dipole case ( $1/R^3$ ). (b) is  $\Delta\phi/\pi$  as a function of  $\langle \varepsilon_{\min} \rangle / \varepsilon_0$ , where  $\varepsilon_0$  is the pair energy of two excited atoms separated by  $R_b$ . The solid line is for the many-atom case. The dot indicates a phase shift of  $0.9\pi$ . The dashed line is for the perfect two-particle case, where the two atoms are in the centre of each sphere.

correlated that they act as a single two-level system. If we had two isolated groups of atoms each of the same size and density such that each group was perfectly blockaded, then we would have two qubits. If we made both groups such that they both sat within  $R_b$ , then again we would have a single two-level system, but as we move one group outside of this ‘bubble’, pairs of intergroup atoms will no longer interact with each other allowing the possibility of a third level: both groups containing an excited atom. When the largest intergroup pair distance is greater than  $R_b$ , both groups are now independent of each other and we are back to two uncorrelated two-level systems. If they are not too far apart however  $R_{\text{pair,max}} \lesssim R_b$ , most of

the intergroup pairs are still correlated, thus both groups are as well. Being in such a state would be undesirable as it leaves us with neither a single two-level system nor two uncorrelated two-level systems.

A quantum gate takes a state and transforms it to another state. We created two spheres of cold atoms, each of radius  $R_0 = R_b/4$ , separated by a centre-to-centre distance  $D$ . Within each sphere, we randomly placed eight atoms. The two groups of atoms are then subjected to the following sequence of pulses: group 1 is excited by a  $\pi$  pulse, group 2 is excited by a  $2\pi$  pulse and finally group 1 is deexcited by another  $\pi$  pulse. The excited atoms interact via the dipole–dipole or van der Waals interaction, depending on the situation. We varied the mean interaction energy between the two groups by increasing  $D$ . In the ideal case, we can represent each group as a two-level system, so the initial state is the ‘ground’ state  $|gg\rangle$ . When the first group is excited by a  $\pi$  pulse  $|gg\rangle \rightarrow -i|eg\rangle$ . If both groups are independent of each other then a  $2\pi$  pulse will take  $-i|eg\rangle \rightarrow i|eg\rangle$ , but if the groups are both within  $R_b$  then it is impossible to excite the second atom and this pulse leaves the state unaffected:  $-i|eg\rangle \rightarrow -i|eg\rangle$ . The final  $\pi$  pulse to the first atom will deexcite it and multiply the state by  $-i$ : for the uncorrelated case  $i|eg\rangle \rightarrow |gg\rangle$  and for the blockaded case  $-i|eg\rangle \rightarrow -|gg\rangle$ . When the groups are independent, there is no accumulated phase shift; the sequence of pulses leaves the original state unchanged. When the system is blockaded, a phase shift ( $\Delta\phi$ ) of  $\pi$  is acquired, making a phase gate [9].

The top plot in figure 4 shows the phase shift  $\Delta\phi/\pi$  as a function of the average maximum intergroup pair distance,  $\langle R_{\max} \rangle$ , divided by the blockade distance. As  $D$  is increased, the distance between the two farthest pairs will also increase beyond  $R_b$ . This allows for the possibility of more than one atom to be excited, thus introducing an error into the phase shift. The solid line in figure 4(a) is for the vdW case and the dashed line is for the dipole–dipole interaction. The rapid  $1/R^6$  scaling of the vdW interaction can be seen in the steep drop of the phase shift with increasing  $\langle R_{\max} \rangle$ . As expected, when  $\langle R_{\max} \rangle$  is small  $\Delta\phi/\pi$  approaches 1 and when  $\langle R_{\max} \rangle$  is large  $\Delta\phi/\pi$  tends to 0. With every intergroup distance, an intergroup pair energy can be calculated; so with each average maximum intergroup pair distance there is an associated average minimum intergroup energy,  $\langle \varepsilon_{\min} \rangle$ , where  $\varepsilon = V\tau/\hbar$ . The solid line in figure 4(b) is  $\Delta\phi/\pi$  as a function of  $\langle \varepsilon_{\min} \rangle/\varepsilon_0$ , where  $\varepsilon_0$  is the pair energy of two excited atoms separated by  $R_b$ . The dot indicates a phase shift of  $0.9\pi$ . The dashed line is for the perfect two-particle case, where the two atoms are in the centre of each sphere. If a phase error of less than 10% is desired, then the average minimum pair energy must be greater than about 2.5. If a phase error of less than 5% is required, then  $\langle \varepsilon_{\min} \rangle > 3.5$ . The difficulty in reducing the error is evident in the flatness of the curve in figure 4(b) as  $\Delta\phi/\pi$  goes to 1.

## 7. Conclusion

By solving for the many-body wavefunction, we were able to calculate many useful quantities such as the 2D two-particle correlation function which shows the angular dependence of the first-order dipole–dipole interaction. When using the dipole–dipole interaction to investigate the  $Q$  parameter or anything else that requires a well-defined blockade region, special care is needed to make sure that the critical angle  $\theta_{jk} \approx 55^\circ$  is unattainable to pairs of atoms. We also calculated the Mandel  $Q$  parameter, a useful quantity for measuring the degree to which a gas is blockaded. The non-excited atoms within a blockade region still affect atoms outside  $R_b$ ; thus even when few atoms are excited and the gas is dense enough, the system is still correlated. The  $Q$  parameter can also be used to indicate how many two-level systems the gas has been reduced to. If atoms are placed on a one-dimensional lattice and excited to the maximum number excited, the average of the maximum number excited grows smoothly as a

function of the lattice length. The size of  $R_b$  can however be seen if the probability of finding  $N_e$  is plotted as a function of  $L$ . Since we solved for the wavefunction, we were able to examine the use of groups of blockaded atoms as phase gates. We calculated the phase accumulated during a sequence of pulses and generated the errors acquired by a non-perfect phase gate as a function of the interaction energy. In order to operate a phase gate that returns  $\Delta\phi > 0.9\pi$ , a rather large interaction energy is required.

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