Many-body wave function in a dipole blockade configuration

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We report the results of simulations of the many atom wave function when a cold gas is excited to highly excited states. We simulated the many body wave function by direct numerical solution of Schrödinger's equation. We investigated the fraction of atoms excited and the correlation of excited atoms in the gas for different types of excitation when the blockade region was small compared to the sample size. We also investigated the blockade effect when the blockade region is comparable to the sample size to determine the sensitivity of this system and constraints for quantum information.

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Recently, a proposal was made to use the dipole-dipole interactions between highly excited atoms for fast quantum gates [1] and for a dipole blockade [2]. Two recent experiments [3,4] have found suppression of laser excitation of cold atoms from small initial states into highly excited states when the laser is on resonance. The suppression arises because the pair energy between two excited atoms is relatively large and can shift the two excitation state out of resonance. Clearly the pair "energy shift" depends on the separation between the atoms. Thus, the probability for finding an excited atom a distance R from another excited atom depends on the properties of the excitation laser, the density of the atomic gas, and the form of the interaction between the atoms. This implies interesting correlations can be imprinted on a gas using an uncomplicated laser pulse.

In addition to computing many body effects, we can use the exact wave function to check simpler models. Reference [3] gave a simple model for the excitation of a gas where the atoms interact through a van der Waals potential. This mean field model can be numerically solved very quickly since it is essentially a one atom calculation that accounts for the energy shift from other excited atoms. The model gave good agreement with the measurements in Ref. [3]. However, some of the experimental parameters were uncertain and the fraction of atoms excited versus laser intensity is a simple function. We show below that this simple model works moderately well for larger laser power. Unfortunately, the mean field model does not give information about the spatial correlation between excited atoms.

In this paper, we report the results of the direct numerical solution of the many atom wave function. For the comparisons, we choose situations similar to those described in recent experiments [3,4] so that all of the physical parameters are experimentally reasonable. The purpose of this paper is to show that in some cases it is possible to numerically solve for the many atom wave function in a manner where the convergence (or lack of it) can be checked; all calculations were performed on a PC with 512 Mb RAM. The wave function can be used to compute many properties of the system, including the number of Rydberg atoms excited ($\langle n_r \rangle$), the positional correlation between the Rydberg atoms, the spread in the number of Rydberg atoms characterized by $Q=(\langle n_r^2\rangle - \langle n_r\rangle^2 - \langle n_r\rangle)/\langle n_r\rangle$, etc. A second purpose is to check the accuracy of simpler mean field models. A third purpose was to investigate the blockade effect when the sample size is comparable to the blockade region. We can answer where the excited atom will likely reside in a finite sample and how sensitive the coherence is to the fraction of the region that is blockaded. Except where explicitly noted, atomic units will be used throughout this paper.

We focus on the major effects that arise due to atom-atom interactions so we will ignore some of the complications of actual systems. We will treat each atom as a two-level system with one level being small and tightly bound and the other level being a Rydberg state. The atoms only interact with the laser and with each other through a two-atom potential when they are both in the Rydberg state. The atoms will be taken to be fixed in space during the laser pulse which will be a good approximation if the pulse is less than a couple 100 ns. The system will be assumed to start with all atoms in the tightly bound state. In terms of the Pauli spinors, the Hamiltonian can be written as

$$H = \sum_j H_j^{(1)} + \sum_{j<k} V_{jk} \frac{1}{2}(1+\sigma_z)_j \frac{1}{2}(1+\sigma_z)_k,$$

$$H_j^{(1)} = -\Delta\omega(t)\frac{1}{2}(1+\sigma_z)_j + \frac{\mathcal{S}}{\tau} e^{-t^2/\tau^2}\sigma_{x,j}, \qquad (1)$$

where $(1+\sigma_z)/2$ is 1 when the atom is excited and 0 otherwise, V_{jk} is the pair interaction between Rydberg states for atoms j,k, $\Delta\omega(t)$ is the detuning of the laser (which could be time dependent if there is a chirp), τ is proportional to the time width of the pulse, and $\mathcal{S}$ is the laser amplitude. This equation uses the rotating wave approximation. When the laser is exactly on resonance [$\Delta\omega(t)=0$], the probability an atom will be excited equals $\sin^2(\sqrt{\pi}\mathcal{S})$ when the blockade effect is negligible. In Ref. [5], we showed excitation coherence is maintained as long as the atoms do not move, either due to their initial velocity distribution or from the acceleration by potentials.

For the recent experiments [3,4], the potential can be approximated by a van der Waals interaction $V=-C_6/R^6$. Other states could give dipole-dipole interactions $V\propto 1/R^3$. Because the atoms are excited from a gas, we randomly distribute the atoms in space and average the results from many

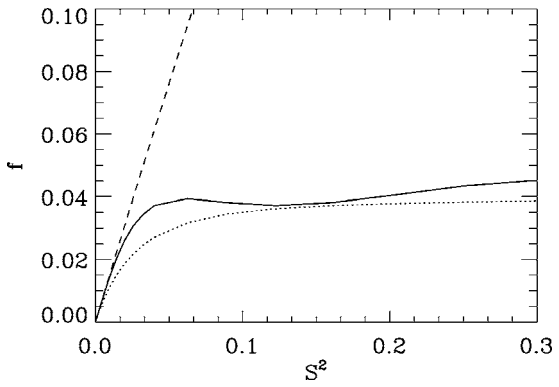

FIG. 1. The fraction of atoms excited versus the square of the laser amplitude $\mathcal{S}$. The dashed line is the single atom result, the solid line is the "exact" result from the many atom wave function, the dotted line is from the mean field model of Ref. [3]. At the end of the range, the dipole blockade effect reduces the fraction of excited atoms by a factor of 8.

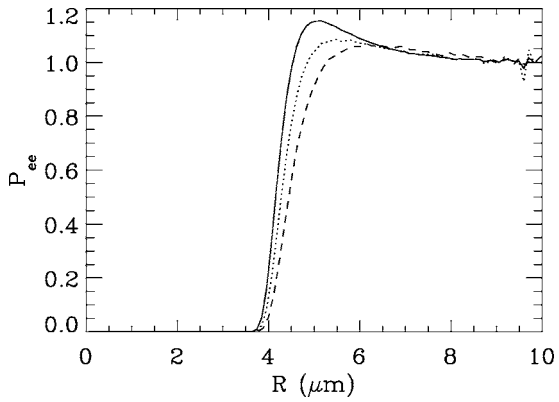

FIG. 2. The pair correlation function between Rydberg atoms versus the distance between the atoms for the parameters used in Fig. 1. The solid line is for an amplitude $\mathcal{S}=0.06$, the dotted line is for $\mathcal{S}=0.10$, and the dashed line is for $\mathcal{S}=0.14$. The fraction of atoms excited divided by the fraction excited with pair interaction turned off is 0.994, 0.95, and 0.85.

random placements of the atoms. We control the errors due to statistical fluctuations in the atom placement by increasing the number of separate runs.

We performed calculations for parameters similar to the experiment reported in Ref. [3]. We used a density of 65×10^9 cm^{-3}, a width $\tau=7.3$ ns, and a detuning $\Delta w(t)=-\sqrt{3}t/\tau^2$ given by laser chirp. We used a pair energy given by $V(r)=-C_6/r^6$ with $C_6=2.64\times10^{22}\times7/60$. In Fig. 1, we show the fraction of excited atoms excited versus the square of the laser amplitude. The probability for exciting a single atom is proportional to the square of the amplitude over most of this range. The models that include the atom-atom interaction show a significant blockade effect; the many atom excitation probability is reduced by a factor of ~8 at the largest laser intensity. Our tests showed that the excitation fraction was clearly converged even at the largest intensity in Fig. 1 so that we could have obtained results for even larger fields.

The strength range is large enough so that the fraction of excited atoms for the full wave function has plateaued with increasing field strength. This behavior is substantially different from what would occur for coherent excitation of a single blockaded wave function. In that case, the wave function has a Rabi oscillation with a frequency that is the square root of the number of atoms larger than the single atom case [2]. The statistics of the number of excited atoms also shows the blockade effect. When the blockade is important, we find that $\langle n_r^2\rangle-\langle n_r\rangle^2$ is much smaller than from Poisson statistics ($Q<0$) [6,7]. For the case of Fig. 1, the mean field model of Ref. [3] does not match the results of the full calculation at smaller laser intensity, but it does give a plateau with roughly the correct number of excited atoms. The inaccuracy at smaller intensities appears to arise from the fact the mean field model of Ref. [3] overestimates the atom-atom interaction when fewer atoms are excited; the atoms at the edge of the sphere (in this model) interact too strongly with the mean excitation outside of the sphere.

To obtain a clearer idea of the blockade effect, we computed the correlation function of atomic excitation from our full wave function. In Fig. 2, we show this correlation function for three laser intensities. The correlation function is defined to be the probability that two atoms separated by a distance R are both excited divided by the square of the probability an individual atom is excited. When the excitation is uncorrelated, then the correlation function is 1. The correlation function is hard to calculate accurately; the average number of excited atoms can be calculated with over an order of magnitude less effort. As expected, the correlation function is essentially zero for small separations due to the blockade and approaches 1 at large distances where the atoms are uncorrelated. For the parameters of Fig. 1, a sphere with a radius 3.7 μm contains ~14 atoms. The correlation function shows a larger region of blockade at higher laser intensities because the mean field from many excited atoms adds to the pair energy shift which gives a larger detuning. Surprisingly, the correlation function is larger than 1 for a range of distances just outside of the blockade region. The effect is strongest for weak excitation. This is due to the chirp of the laser which gives negative detuning after the peak of the laser pulse; a negative detuning is in the direction of the pair energy shift and thus allows a resonant transition. Calculations with no chirp do not show a region where the correlation is larger than 1 for the current parameters. Also, the chirp in Fig. 1 causes the blockaded region to be somewhat smaller than when the laser is unchirped.

We performed calculations for parameters similar to the experiment reported in Ref. [4] except the time width of the laser pulse was chosen to match the reported band width of the experiment. We used a density of 2×10^9 cm^{-3}, a width $\tau=37.5$ ns, and a constant detuning with no laser chirp. We used a pair energy given by $V(r)=-C_6/r^6$ with $C_6=-4.97\times10^{22}$. We found that linewidth and position did not strongly depend on the blockade effect. These results clearly differ from those reported in the experiment (Ref. [4], Fig. 2). In the experiment, the number of excitations versus detuning gives a much larger width when the atoms are blockaded. This is probably due to the long laser pulse width (~20 μs) in the experiment. For such a long pulse, the at-

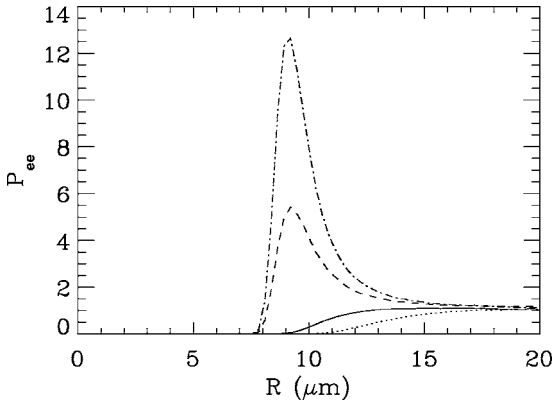

FIG. 3. The pair correlation function between Rydberg atoms versus the distance between the atoms. When the laser amplitude $\mathcal{S}=0.2$, the solid line is for 0 detuning, the dotted line is for a detuning of $-2/\tau$, and the dashed line is for a detuning of $2/\tau$. The dot-dashed line is for a detuning of $2/\tau$ and $\mathcal{S}=0.1$.

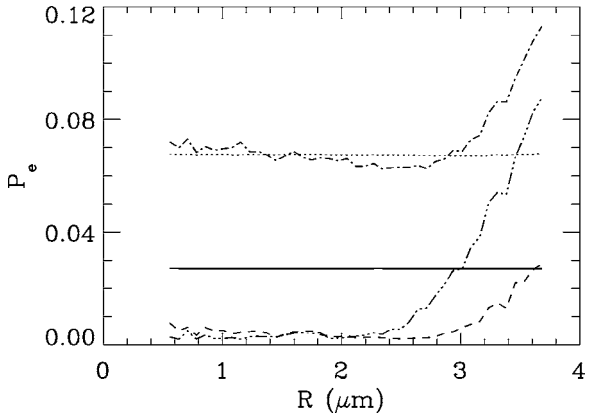

FIG. 4. The probability for exciting an atom inside of a finite spherical region as a function of distance from the center; there are 14 atoms in the sphere and the blockade distance for infinite sample is 6.6 μm. The solid line is for $\mathcal{S}=0.1$, the dotted line for 0.2, the dashed line is for 0.5, the dot-dash line is for 0.7, and the dot-dot-dot-dash line is for 1.0. Note that the center of the sample shows a stronger Rabi oscillation than the edge. At high intensity, the excitation are most likely to be found near the edge of the sphere.

oms can move substantial distances compared to the spacing. Therefore, we expect there are many interesting physical processes occurring in this experiment in addition to the pure blockade effect we are investigating in this paper.

In Fig. 3, we show the correlation function for several detunings. Note that when the detuning is in the opposite direction of the van der Waals shift, the blockaded region becomes larger and the transition to the uncorrelated limit is over a larger distance compared to when the detuning is 0. When the detuning is in the direction of the van der Waals shift, atom pairs are preferentially excited at separations that give a two photon resonance. This is an exaggerated form of the peak seen in Fig. 2 at low power which was due to the chirp. Note that the effect is even stronger when the laser intensity is less. The relative increase in the peak correlation with decreasing intensity is due to the fact that at low intensities very few atoms are excited so that the main process is a correlated two photon absorption, but only for resonant separation. At higher intensities, the first step makes an excited pair of atoms with the resonant separation; in the next step, one or more extra atoms can be excited if the sum of the van der Waals shifts matches the detuning. However, these extra atoms will not be at the peak separation for *all* of the other excited atoms.

In using the dipole blockade effect for quantum information, the sample needs to respond coherently. If the blockade region is much larger than the sample size, this will clearly hold. It is likely that the first experimental attempts will be for systems where the size of the sample and the blockade region will have comparable size. Thus, it is important to study the blockade for this situation. We investigated the case where a fixed number of atoms were randomly placed inside of a sphere. We present results for 14 atoms in a sphere of radius 3.72 μm with the C_6 coefficient of Fig. 1. We tuned the laser to resonance and removed the chirp, $\Delta\omega=0$ to give the largest blockade region. For τ of 73 ns, the blockade region (defined to be where the correlation function reaches 1/2) is roughly 6.6 μm, approximately 90% of the sample diameter.

There are two clear signatures of a strongly blockaded system: (1) the number of excited atoms oscillates between 0 and 1 and (2) the probability for an atom to be excited does not depend on its position in the sample. While (1) is easier to measure experimentally, (2) contains more information. In Fig. 4, we show the fraction of excited atoms as a function of distance from the center for several laser strengths. Notice that only for the smallest strengths is the excitation fraction independent of position. It is clear that the excitation fraction near the center oscillates more strongly than near the edge. Defining the contrast to be (MAX−MIN)/(MAX+MIN), the center has a contrast >0.9 while the edge is ~ 0.3 for $\mathcal{S}>0.6$; the minimum $\langle n_r\rangle$ for the whole sample is ~ 0.15 at one blockade Rabi period and ~ 0.45 at two periods. There is a substantial probability for having two excited atoms in the sample at larger $\mathcal{S}$, but the probability for three excited atoms is less than 1% even at the highest laser strengths. Thus, only one extra excitation almost completely destroys the blockade after one Rabi flop. Increasing τ to 146 ns increases the radius of the blockade region to 7.4 μm which is the sample diameter. At one blockade Rabi period $\langle n_r\rangle=0.016$ and is ~ 0.09 at two periods; the sample contrast is >0.8 between the first and second blockade Rabi period.

We now describe some of the physics of the system that allow an enormous reduction in numerical effort for the *infinite* systems. Since the correlations only extend over a finite range, we only solve for atoms in a limited, cubical volume with the number of atoms in a simulation being ρL^3 where ρ is the density of atoms. To help reduce errors from the finite size of the cube, the interaction between atoms is computed using wrap conditions. We also include the mean field from excited atoms outside of the cube. For the van der Waals potential, the energy shift for an atom excited at the center of a cube due to a uniform distribution of excited atoms *outside* the cube is approximately equal to $\varepsilon(t)\simeq -P(t)20C_6\rho L^{-3}$, where $P(t)$ is the fraction of excited atoms at time t; $P(t)$ is averaged from the many runs with different random place-

ment of atoms. Roughly speaking, the cube needs to be large enough to cover the region of correlation.

Even with the finite volume simplifications, the direct solution of the many atom wave function is apparently impossible. In many of the cases we simulated, between 30–160 atoms (10^9–10^{48} states) were needed to converge the correlation function. It is not possible to solve Schrödinger's equation on an average PC with more than 10^8 states. We overcame this difficulty in two stages. The most important simplification used the blockade effect to choose the states needed in the calculation. We replaced strongly blockaded atoms with pseudoatoms using the following recursion. Start with the real atoms distributed at their random positions with the separation of the atoms i and j given by R_{ij} and the "weight" of every atom W_i set to 1. Now recursively reduce the number of "atoms" from the physical number of atoms N to the number of pseudoatoms with the 3 steps: (1) find the pair i,j with the smallest separation, (2) replace the two atoms, with an atom at the center of mass position $\vec{R}_i=(W_i\vec{R}_i+W_j\vec{R}_j)/(W_i+W_j)$ taking appropriate care of the wrap boundary condition, and (3) set new $W_i=W_i+W_j$ and remove atom j from the simulation. When the simulation is run, the pseudoatom i has an interaction with the laser field that is a factor of $\sqrt{W_i}$ larger than the single atom strength and the pair shift is computed from the positions of the pseudoatoms. Errors due to the forced correlation of near atoms can be controlled by increasing the number of pseudoatoms which decreases the number of atoms that compose each pseudoatom.

Although this gave a great reduction in most cases, it was not enough for some of the situations where the correlation extended over many atoms. We implemented a further reduction based on the obvious realization that only a small fraction of the states are needed because only a fraction of the atoms are excited. Therefore, an upper limit for the number of Rydberg atoms n_r can be chosen and the number of states needed for an N atom wave function is $1+N/1!+N(N-1)/2!+\cdots+N!/[n_r!(N-n_r)!]$. For example, only 536 155 states are needed when the number of atoms is 24 and the maximum number of excitations is 7 (instead of the full 17 million states).

Using 64 atoms that were reduced to 16 pseudoatoms (with up to six excitations) produced accurate results over the intensity range showed in Fig. 1; convergence was checked by also performing calculations for 100 atoms that were reduced to 25 pseudoatoms (with up to 7 excitations) and 64 atoms reduced to 32 (with up to six excitations).

In conclusion, we were able to directly solve for the many atom wave function by using several physical properties to reduce the size of the state space. We were able to calculate both the fraction of excited atoms and correlation properties of the wave function in a manner that allowed us to ensure convergence. We used this tool to investigate two systems similar to those investigated in recent experiments and a finite sized system that could be the starting point for quantum information experiments. From the wave function, we found correlation properties of the systems that could not be measured in the experiments. We note that it is possible to experimentally probe the pair correlation function to some extent. For example, Rydberg gases spontaneously ionize due to collision between pairs of Rydberg atoms; the distribution of distances between pairs of Rydberg atoms affects the time dependence of this ionization. Also, the frequency dependence of microwave absorption will also depend on the distribution of distances between pairs of Rydberg atoms. Our calculations on finite size systems shows that the blockade region must fully cover the system for a clear effect to occur.

There are many other properties and systems that we can investigate by directly solving the wave equation for the dipole blockade configuration. We end this paper with questions whose answers now seem within reach. How is the fraction of blockaded atoms correlated with the distribution of number of excited atoms? (Preliminary results suggest $-Q$ equals the fraction of excited atoms times the number of blockaded atoms.) What are the correlation properties of this system at large laser intensities? Is there correlation between local density fluctuation and excitation? When does atom motion become important for blockade excitation? The direct solution of the wave equation opens many new possibilities, most of which have not been mentioned here.

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