

Numerical study of two-body correlation in a 1D lattice with perfect blockade

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Abstract. We compute the dynamics of excitation and two-body correlation for two-level ‘pseudoatoms’ in a one-dimensional (1D) lattice. We adopt a simplified model where pair excitation within a finite range is perfectly blocked. Each superatom is initially in the ground state, and then subjected to an external driving laser with Rabi frequency satisfying a Poissonian distribution, mimicking the scenario in Rydberg gases. We find that two-body quantum correlation drops very fast with the distance between pseudoatoms. However, the total correlation decays slowly even at large distance. Our results may be useful to the understanding of Rydberg gases in the strong blockade regime.

Recently, there have been many experimental efforts in investigating Rydberg gases [1]–[7], spurred largely by fast developments in laser cooling and trapping. In such systems, the dipolar interaction between two nearby atoms will shift the pair excitation out of resonance with the driving laser. Local excitation is then greatly suppressed, showing the well-known phenomenon of dipole blockade. It is an important mechanism responsible for the explanation of many-body effects such as spectral line broadening [1, 2] and the expected sub-Poissonian atom counting statistics [4, 8, 9]. It is also proposed to utilize dipole blockade to implement quantum gates useful in quantum computation and information [10, 11]. To date, there have been many theoretical proposals and numerical simulations in exploring the excitation dynamics and coherence properties such as pair correlation and number correlation, which demonstrate the important role that dipole blockade played in these systems.

Previous investigations of Rydberg gas have focused on the mean number of excitations and how the excitations are correlated in a gas. However, there has not been a study of genuine quantum correlation. This paper will discuss other useful information that can be extracted from

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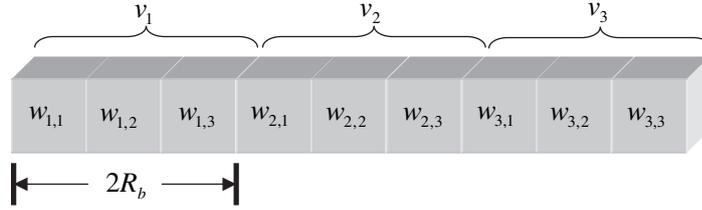


Figure 1. A schematic view of partitioning 3 superatoms into 9 pseudoatoms. Each v_k ($k = 1, 2, 3$) represents a superatom which is further divided into 3 pseudoatoms $w_{k,\alpha}$ ($\alpha = 1, 2, 3$).

the wavefunction, especially the two-body quantum correlation and total correlation (including classical correlation). As we will see later, two-body correlation is another important quantity for characterizing such systems. To investigate correlation properties, we are mainly interested in the following two questions. Firstly, in such systems, how does correlation behave as the excitation begins to build up? Secondly, which correlation is more important? It has been shown that a mean field approach is not appropriate in dealing with correlation and a full quantum calculation is necessary [12]. However, the direct simulation of correlation is still absent due to numerical complexities in real Rydberg gases.

We first consider the scenario as in current experiments where Rydberg atoms are confined in a volume \mathcal{V} and driven by a laser. In the spirit of the dipole blockade model, we can divide \mathcal{V} into equally sized regions $\mathcal{V} = \cup_k v_k$ with each region approximated as a sphere of blockade radius R_b . We follow the usual notation and call the ensemble of atoms in each region v_k a ‘superatom’ [13]. For van der Waals interaction and a narrow band laser, R_b is determined from $C_6/R_b^6 = \Omega$, where C_6 is the van der Waals coefficient in the atomic unit and Ω is the Rabi frequency of the driving laser. Rydberg atoms are randomly distributed in \mathcal{V} so that the number of atoms in each v_k is in general different. For example, in the homogeneous case, the atom numbers in each superatom follow a Poissonian distribution with the same mean atom number. Such a picture is useful in explaining certain experimental results, e.g. the population dynamics under a driving laser. In this case, each superatom evolves with different Rabi frequencies. This leads to a fast and almost linear increase in the initial stage and saturation in the long time. However, such a model is not so interesting in showing the two-body correlation properties because correlation between different superatoms is apparently 0. Therefore, a proper modification to the superatom model is necessary in order to give nontrivial information on two-body correlation.

In this paper, we discuss an elongated Rydberg gas whose transverse size is smaller than R_b . This allows us to treat the Rydberg gas as a quasi-one-dimensional (1D) system. The advantage is twofold. On the one hand, the edge effect in numerical simulation is smaller and the results converge relatively faster than those in higher dimensions with the same atom number. On the other hand, it permits an easier readout of the quantum state for an ensemble of atoms in any region along the longitudinal direction. Similar to the 3D case, we divide such a quasi-1D gas into a collection of superatoms aligned along the longitudinal direction. We investigate the two-body correlation by further dividing each superatom (v_k) into smaller subregions labeled as $w_{k,\alpha}$, i.e. $v_k = \cup_{\alpha=1}^{N_w} w_{k,\alpha}$. The center of $w_{k,\alpha}$ is denoted as $r_{k,\alpha}$. The number of partitions in each v_k , labeled as N_w , is assumed the same, $\forall k$. For the interest of this paper, we term each subregion $w_{k,\alpha}$ as a ‘pseudoatom’ located at position $r_{k,\alpha}$. In figure 1, we give a schematic view of partitioning three superatoms into nine pseudoatoms. The subscripts k and α can be further combined

into a single one by relabeling them as in a spin chain. Interaction between two pseudoatoms on sites j and k are assumed to be a van der Waals interaction with the distance $|r_j - r_k|$. This approximation neglects the position variance of excitation in each pseudoatom. By partitioning each superatom into more pseudoatoms, the error can be reduced. Different from the case of nearest neighboring superatoms (with a distance $2R_b$), where the interaction is usually ignored, we can see that nearest neighboring pseudoatoms (with a distance of a fraction of R_b) interact much more strongly so all of the pseudoatoms are correlated analogous to a spin chain.

Due to the R^{-6} dependence of interaction, the transition from blockade to no blockade has a narrow width of R . This gives us the motivation to assume a perfect blockade with pseudoatoms within a certain distance and completely no blockade outside it. From the many body point of view, the introduction of this approximation allows us to concentrate on the much simpler short-range interaction rather than the long-range interaction. It not only lets us see the effect due to pure blockade, but also greatly reduces the needed basis which makes the numerical simulation in a much larger system possible. The validity of this approximation will be discussed in the later part of this paper. Because of this type of partition for a superatom, the maximal number of pseudoatoms that can be blocked is just the maximal distance between two pseudoatoms j and k which have an interaction $V_{j,k}$ much larger than the Rabi frequency Ω , i.e. $\max_{j,k}\{j - k | V_{j,k} / \Omega > \eta\}$. Besides the vagueness of this definition, in practice we choose $\eta = 6$. A little algebra shows that the maximal number of pseudoatoms that can be blocked is given by $\max_{k=0,1,2,\dots}\{k | k < 0.37N_w\}$. The first few values are given here: for $N_w = 2, 3, 4, 5, 6, \dots$, the maximal number of pseudoatoms that can be blocked is found to be $0, 1, 1, 1, 2, \dots$, respectively. So the simplest nontrivial situation starts from $N_w = 3$, perfect blockade only between two nearest neighboring pseudoatoms. In this paper, we will limit our discussion to the situation where perfect blockade only exists between two nearest neighboring pseudoatoms.

Because of our approximation, the Hamiltonian can be written as $\hat{H} = \sum_{k=0}^{N-1} J_k \hat{P}^{(k)} \hat{\sigma}_x^{(k)} \hat{P}^{(k)}$, with the projector

$$\hat{P}^{(k)} \equiv \prod_{q=k\pm 1} \frac{1 - \hat{\sigma}_z^{(q)}}{2}, \quad (1)$$

where N is the total number of pseudoatoms. $\hat{\sigma}^{(k)}$ are Pauli matrices for the k th pseudoatom. $J_k = \sqrt{X_k/\lambda}$ is the scaled Rabi frequency for the k th pseudoatom. We are assuming a resonant laser field with a constant intensity. X_k is a random variable satisfying a Poissonian distribution with mean value λ . In this case, λ denotes the average number of Rydberg atoms in a pseudoatom. More explicitly, $\lambda = N_r/N_w$ with N_r the number of Rydberg atoms in a superatom which can be determined from the Rydberg gas density n , the blockade radius R_b and the area in the transverse direction A through the relation $N_r = 2nR_bA$. The underlying motivation for the assumed form of J_k is the number fluctuation and the collective excitation in each pseudoatom [6]. A given set of $\{J_0, \dots, J_{N-1}\}$ is said to define a configuration. Our numerical results are obtained by averaging over many configurations. We note that the Hamiltonian formally describes a nonphysical multi-body interaction, which is of course an effective Hamiltonian constrained by the perfect blockade requirement. All the pseudoatoms are initially in the ground state $|g\rangle^{\otimes N}$, and then subjected to a resonant external laser field. The subsequent dynamics constrained by the perfect blockade are what we are after in this paper.

For nearest neighboring blockade, the maximally possible excitation for all pseudoatoms is found to be $[N/2]$ where $[\cdot]$ denotes the integer part. As a consequence, the number of restricted basis, N_b , is significantly reduced from that of the full basis set. To compute the wavefunction,

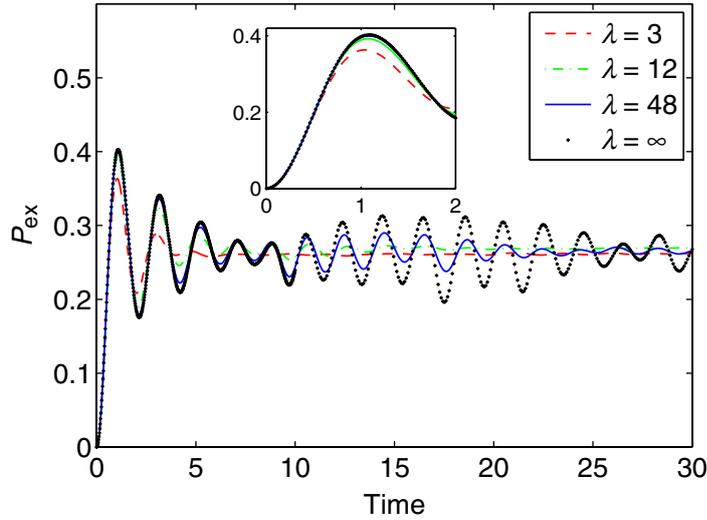


Figure 2. Excitation fraction P_{ex} as a function of time for different λ . The inset shows an enlarged version of initial dynamics.

we expand it in the restricted basis labeled as $|\mu_p\rangle$, i.e.

$$\psi(t) = \sum_{p=1}^{N_b} c_p(t) |\mu_p\rangle, \quad (2)$$

the fraction of excitation is found to be

$$P_{\text{ex}}(t) = \frac{1}{N} \sum_{p=1}^{N_b} |c_p(t)|^2 \langle \mu_p | \sum_{k=0}^{N-1} |e\rangle_k \langle e | | \mu_p \rangle. \quad (3)$$

In figure 2, we show the numerical results of excitation fraction as a function of time for pseudoatom number $N = 16$. The results are obtained by using wrap boundary condition and averaging over 1000 different configurations of $\{J_k\}$. We can see that the overall trends of the curves for different λ are similar. In all cases, P_{ex} first increases almost linearly and overshoots to a maximal value, then oscillates and saturates to about 26%, close to the expected value (25%). It comes from the fact that for two pseudoatoms with perfect blockade, the wavefunction should behave like $\cos(Jt)|gg\rangle + \sin(Jt)(|eg\rangle + |ge\rangle)/\sqrt{2}$, so the total time-averaged excitation for one pair of pseudoatoms is 50%, i.e. 25% for each pseudoatom. It is also obvious that the larger λ , the less fluctuation in J_k , so that we can observe more oscillations. For $\lambda = \infty$, when there is no fluctuation at all, the oscillation period can be estimated from analyzing the spectrum of the Hamiltonian. Labeling the eigenvalues and the corresponding eigenstates as E_α and $|E_\alpha\rangle$ ($\alpha = 1, 2, \dots, N_b$) respectively, we find that there exists a nearly periodic structure in the plot of $|\langle \psi(t=0) | E_\alpha \rangle|^2$ versus E_α . In this case, P_{ex} does not saturate to a fixed value for $N = 16$ pseudoatoms.

The excitation fraction of a physical Rydberg gas can be qualitatively obtained by the mean field approach [3], which is essentially a reduction to the single-atom picture. However, the two-atom correlation, where the off-diagonal terms of the density matrix are important, cannot be simply accounted for from the mean field approach. In the following, we will focus on correlation properties of a reduced two-pseudoatom subsystem from a full quantum mechanical calculation.

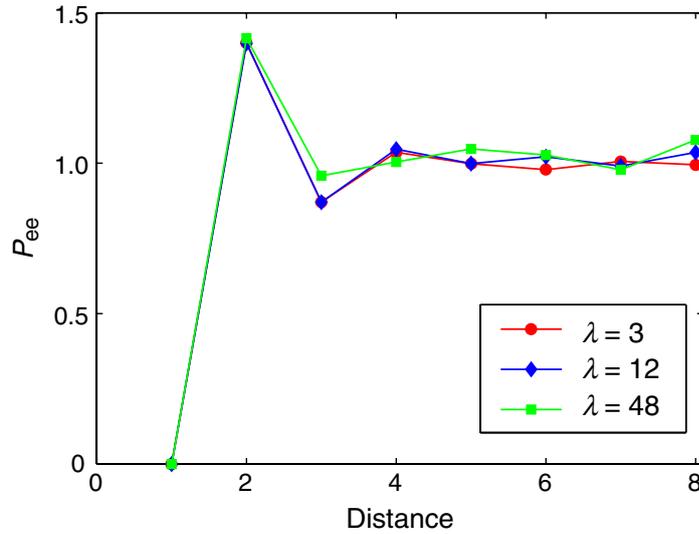


Figure 3. Pair correlation P_{ee} as a function of distance for different λ . Solid lines are a guide to the eye.

The first quantity we will look into is the pair correlation, P_{ee} , at saturation time, which is defined as the ratio of the probability of both pseudoatoms excited divided by the square of probability of single-pseudoatom excitation [12]. In figure 3, we show P_{ee} as a function of distance for different λ . Compared with the results in [12] (see figure 2) which uses a continuous model, our results captures the main physics in a much simpler way. We can see that for both the discrete and continuous model, P_{ee} exhibits similar behavior: it is negligible within a distance and there is a sharp increase after that; at large distance, it saturates to 1, corresponding to no correlation. For all three λ in our calculation, the next to nearest neighbor always has the largest value. This can be interpreted as follows. Assuming the index of the first pseudoatom to be 0, the separation d is simply the label of the other pseudoatom. P_{ee} for $d = 1$ is 0 because pseudoatom 1 cannot be excited once pseudoatom 0 is excited. For $d = 2$, P_{ee} is well above 1. This is because if pseudoatom 0 is in the excited state, then pseudoatom 1 must be in the ground state. Thus pseudoatom 2 is more likely to be in the excited state. Similarly, pseudoatom 3 will be less likely in the excited state, resulting in a value lower than 1. The fast approach to 1 at large distance means that such pair correlation is only short range. We do not present the result for $\lambda = \infty$ due to the non-negligible oscillation even at long enough time.

While the above pair correlation only relies on the diagonal elements of the reduced two-body density matrix, the genuine quantum correlation must be computed from the full reduced two-body density matrix. We use entanglement of formation (EOF) as our measure for quantum correlation [14]. It is related to the so-called concurrence, $C = \max(0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4})$, where λ_i are the eigenvalues of a Hermitian matrix, $R \equiv \sqrt{\rho}(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)\sqrt{\rho}$, in descending order. EOF (ε) is then given by $\varepsilon = h((1 + \sqrt{1 - C^2})/2)$, where $h(x) = -x \log_2(x) - (1 - x) \log_2(1 - x)$. ε gives 0 for separable states and 1 for maximally entangled states.

In figure 4, we show EOF for pseudoatom pairs (0, 1) for different λ . We find that $\varepsilon^{(0,1)}$ shows a similar pattern to the excitation fraction. During the same timescale, they approach a maximal value and then decay slowly. This reflects two simple facts, that entanglement

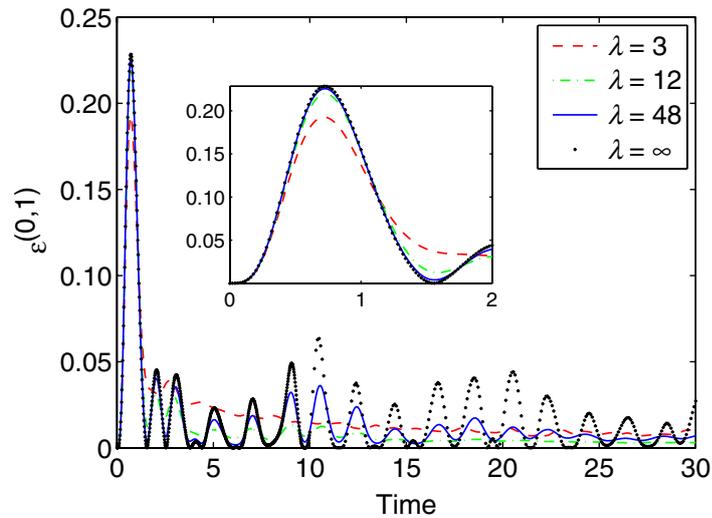


Figure 4. EOF ε as a function of time for different λ . The inset shows an enlarged version of initial dynamics.

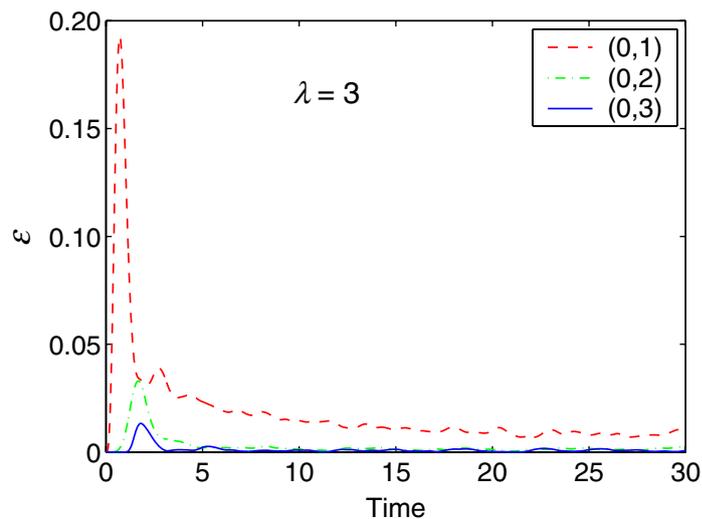


Figure 5. ε as a function of time for different pairs with $\lambda = 3$.

originates from excitation and it is superposed coherently in the initial stage. The behavior of entanglement for other pairs is shown in figure 5. We can see that they again behave in a similar way, although the first peaks are offset in time.

To investigate how entanglement varies with the distance between pseudoatoms, we use the first peak of EOF for different pairs to characterize its dependence on the distance. Our results are shown in figure 6. We note that EOF drops almost exponentially as the distance increases for all λ . Thus, we emphasize an important point here: only nearest neighboring pseudoatoms have relatively large entanglement. Entanglement of other pseudoatom pairs is negligible during the full timescale we investigate. This is consistent with our intuitive understanding that there is no long-range order in such systems.

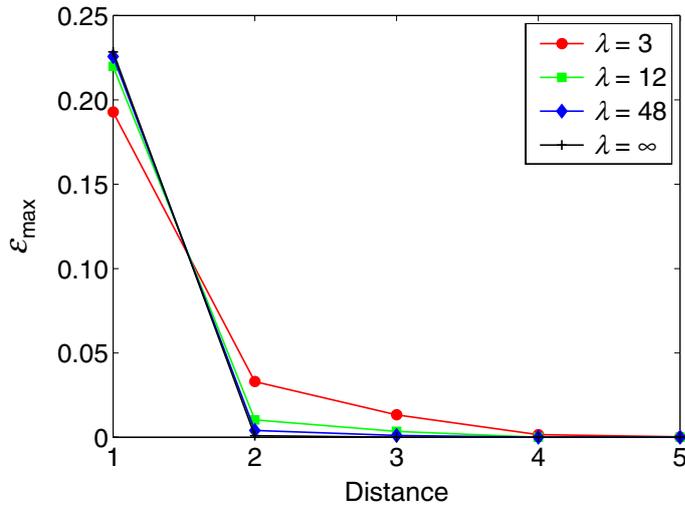


Figure 6. The first peak of EOF as a function of distance for different pairs. Solid lines are a guide to the eye.

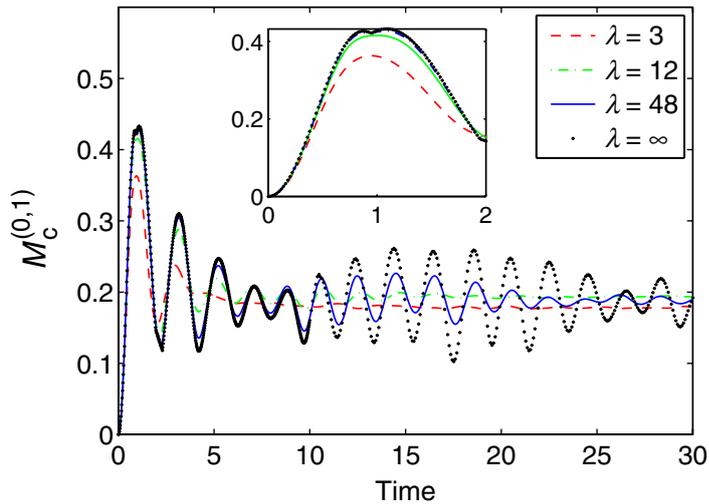


Figure 7. Total correlation of pair (0, 1) as a function of time for different λ . The inset shows an enlarged version of initial dynamics.

We can see that quantum correlation is significant only for nearest neighboring pseudoatoms. However, this is not the case for the total correlation (including classical correlation). To compute the total correlation, we adopt the measure as suggested by Zhou and You [15]. For density matrix $\rho_{(12)}$ of pseudoatoms 1 and 2, it is given by

$$M_c = \frac{2}{3} \text{Tr} |\rho_{(12)} - \rho_{(1)} \otimes \rho_{(2)}|, \quad (4)$$

where $\rho_{(k)}$ is the reduced density matrix of the k th pseudoatom. Different from [15], here the prefactor $2/3$ is chosen so that this measure gives 1 for a maximally entangled state.

In figure 7, we show the total correlation as a function of time for different λ . We again see that they show a similar pattern to EOF. To investigate the distance dependence of total correlation, we show the first peak value of total correlation in figure 8. We can see that total correlation does not drop like a single exponential function with distance as in EOF. Rather

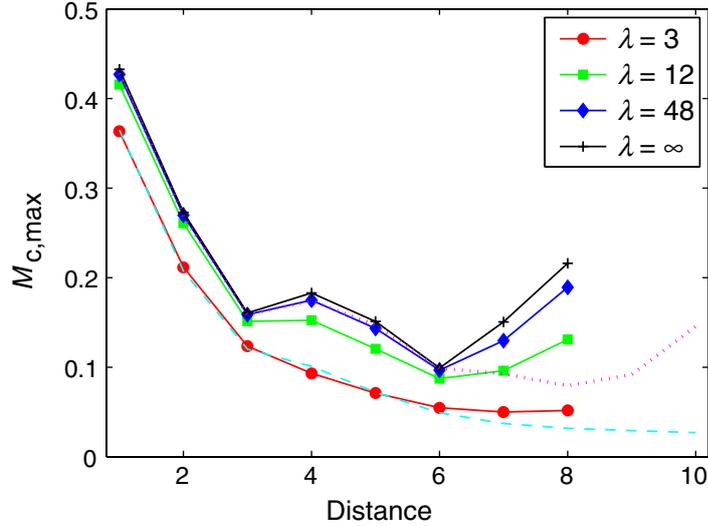


Figure 8. The first peak value of total correlation as a function of distance. Marked curves are for $N = 16$ with corresponding λ shown in the legend. Unmarked curves are for $N = 20$ with the lower (dashed) and upper (dotted) curves corresponding to $\lambda = 3$ and 48, respectively.

interestingly, it does not even decrease monotonically with increasing distance. A simulation with $N = 20$ atoms shows similar behavior with distance. We find that they give almost identical results for several initial distances. However, close to the middle point of the lattice (distance $N/2$), those values of $N = 20$ have correspondingly lower values than $N = 16$. Therefore, such non-monotonicity will become negligible for $N \rightarrow \infty$, i.e. a finite size effect. We conclude that although quantum correlation is not important in most cases, the total correlation cannot be simply ignored, i.e. there is non-negligible classical correlation in such systems. It is necessary to include not just nearest neighboring pseudoatoms when considering correlation-related properties.

The extension of our results to higher dimensions seems difficult due to the computational limitation. For 2D configurations and nearest neighbor blockade, we can only simulate up to 5×5 square lattice. Without presenting more figures, we briefly discuss our results. Our major results for 1D still hold in 2D configurations. We find that EOF shows similar patterns but drops even faster as distance increases. This is possibly due to the fact that in 2D, as more neighboring pseudoatoms are involved, the fluctuation is more intensive than that in 1D. In addition, the corresponding pair entanglement is found to be smaller than that in 1D. Thus, we conjecture that the pair entanglement is even smaller in a 3D cubic lattice.

Before concluding, we want to justify the validity of our simplified Hamiltonian. We will show that the fast decay of entanglement with distance is not an artifact of the assumed short-range interaction. To confirm this point, we carry out simulations using the long-range interaction,

$$\hat{H}' = \sum_k J_k \hat{\sigma}_x^{(k)} + \sum_{j < k} \frac{D}{|j - k|^6} \frac{1 + \hat{\sigma}_z^{(j)}}{2} \frac{1 + \hat{\sigma}_z^{(k)}}{2}, \quad (5)$$

where J_k takes the same form as in the Hamiltonian \hat{H} . The dimensionless parameter D quantifies the interaction strength between two nearest neighboring pseudoatoms. Because we

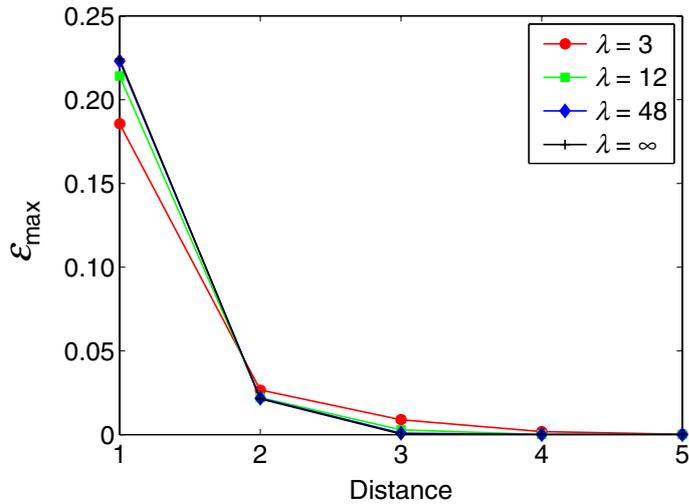


Figure 9. ε_{\max} as a function of distance for $N_w = 5$ with nearest neighboring blockade.

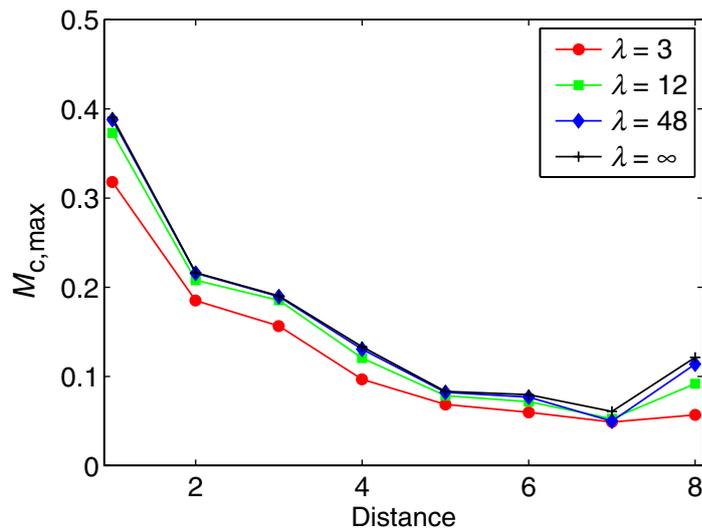


Figure 10. $M_{c,\max}$ as a function of distance for $N_w = 5$ with nearest neighboring blockade.

always use the distance between two nearest neighboring pseudoatoms as the length scale, D also depends on N_w , i.e. the decrease in the distance is equivalent to the increase in the interaction strength. We carry out similar calculations by using the full basis of \hat{H}' . Selected results for $N_w = 5$ with nearest neighboring blockade are shown in figures 9 and 10, for ε_{\max} and $M_{c,\max}$ as a function of distance, respectively. We find that the main features by using \hat{H}' are qualitatively reproduced by the simplified Hamiltonian \hat{H} , which leads us to conclude that the behavior of entanglement with distance is not an artefact of short-range interaction in the simplified Hamiltonian \hat{H} . And for the total correlation, the overall shape of the curves remains the same. More importantly, the total correlation does not drop as fast as entanglement with distance, which provides further evidence that our simplified model captures the main physics.

We emphasize that this calculation not only justifies our simplified model, but also means that those effects in figures 6 and 8–10 are mostly due to blockade, which shows that the long-range interaction is actually not so important to correlation properties.

In conclusion, we have performed full quantum calculations on correlation properties for pseudoatoms in a 1D lattice structure with perfect blockade. By comparing the results from a reduced basis and a full basis calculation, we justify the validity of the simplified Hamiltonian for perfect blockade among pseudoatoms. This agreement also means that single- and two-particle correlation properties (e.g. average excitation and correlation) are determined mostly by the pure blockade effect. From numerical simulation, we find that there are both quantum and classical correlations accompanying the building up of atomic excitation. Our results show that two-body entanglement is only important for nearest neighboring pseudoatoms and it drops exponentially fast with the distance between them even when there is no fluctuation in the system. However, the total correlation decays much more slowly with distance, showing the system in this paper is mostly classically correlated. As a simple extension to higher dimension, we compute our model system in a 2D 5×5 square lattice. We find 2D results agree qualitatively with those of 1D. From the theoretical point of view, our findings imply that a better description of Rydberg gas beyond the mean field or superatom picture should also at least take classical correlation into consideration. We hope that our study can be helpful to the understanding of Rydberg gases in the strong blockade regime.

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