Collective many-body interaction in Rydberg dressed atoms

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We present a method to control the shape and character of the interaction potential between cold atomic gases by weakly dressing the atomic ground state with a Rydberg level. For increasing particle densities, a crossover takes place from a two-particle interaction into a collective many-body interaction, where the dipole-dipole/van der Waals Blockade phenomenon between the Rydberg levels plays a dominant role. We study the influence of these collective interaction potential on a Bose-Einstein condensate, and present the optimal parameters for its experimental detection.

The remarkable success of ultra-cold atomic gases in exploring quantum phenomena from the weakly interacting regime to strongly correlated many-body physics is founded in the microscopic understanding of the two-body interaction potential, and the possibility to control it by external fields. Several tools are nowadays available to control the strength and shape of the interaction potential with the most prominent examples being magnetic and optical Feshbach resonances \cite{1–4}, atomic gases with large magnetic dipole moments \cite{5}, as well as the recently realized polar molecules \cite{6}. An alternative class of strong interactions appears between atoms excited into a Rydberg state \cite{7}. In this letter, we show that the shape and character of the interaction potential between ground state atoms can be altered by dressing them with a Rydberg level giving rise to a collective many-body interaction.

The optical dressing of ground state atoms with an excited electronic state has extensively been studied in the past in the context of “blue shield” for the suppresion of inelastic collisions \cite{8}. Motivated by recent experimental progress in manipulating Rydberg atoms also in the ultra-cold regime \cite{9}, the possibility of controlling the interaction via Rydberg dressed ground state atoms has been proposed for the dipole-dipole interaction in the strongly interacting regime \cite{10}, and for inducing short range interactions in a Bose-Einstein condensate \cite{11}. In contrast to the earlier proposals \cite{12}, these approaches use a finite detuning in order to reduce losses via spontaneous emission from the excited Rydberg state.

Here, we study the influence of Rydberg dressed interactions on the ground state wave function of a Bose-Einstein condensate. The combination of strong interactions between the Rydberg state and the detuning gives rise to a large effective range of the interaction potential, which exceeds the natural interparticle distance in cold atomic gases. Within this regime, we show that a crossover from a two-particle interaction potential to a collective many-body interaction takes place. This collective many-body interaction appears as a consequence of the dipole/van der Waals blockade extensively studied in the past \cite{13,14}. We provide a description for this collective interaction in a Bose-Einstein condensate and discuss its experimental signatures.

![FIG. 1. (a) Setup for the ground state dressing with the Rydberg level $|r\rangle$ via the intermediate $|p\rangle$ state with the corresponding Rabi frequencies and detunings. (b) Diagram showing the crossover from the two-body interaction potential into the regime with a collective many-body interaction. The crossover line is determined by $\Delta \sim -\Omega^{4/5}$ (red dashed line), which preempts the condition of weak dressing $\Omega \lesssim |\Delta|$.](image-url)

In the following, we are interested in a two-photon coupling of the ground state atoms to a high lying Rydberg state; see \cite{9} for such an experimental setup. Then, the relevant internal structure for each atom is given by a three-level system: the atomic ground state $|g\rangle$ is coupled to the Rydberg level $|r\rangle$, via the intermediate $|p\rangle$ state, see Fig. 1. The Rabi frequency and detuning for the transition from the ground state to the $p$-level is denoted as $\Omega_p$ and $\Delta_p$, and for the transition from the $p$-level to the Rydberg state $\Omega_r$ and $\Delta_r$, respectively. The intermediate $p$-level is far detuned, $\Delta_p \gg \Omega_r, \Omega_p$, and can be adiabatically eliminated. Then the dynamics for a single atom reduces to an effective two level system $H_2 = \hbar \left( \Omega \sigma_z^{(i)} - \Delta \sigma_z^{(i)} \right) / 2$ with the two-photon Rabi frequency $\Omega = \Omega_p/\Delta_p$ and the total detuning $\Delta = \Delta_r + \Delta_p$; here $\sigma_z^{(i)}$ denote the Pauli matrices. In the following, we first derive the two-body interaction potential in the regime with large detuning, i.e., $\Omega \ll |\Delta|$. Then, the ground state atom is weakly dressed with the excited Rydberg level $|+\rangle \approx (1 - \Omega^2/8|\Delta|^2)|g\rangle + \Omega/2|\Delta|r\rangle$ providing a small fraction $f \approx \Omega^2/4|\Delta|^2$ of excited Rydberg atoms. At large distances and in absence of Förster resonances \cite{15}, the interaction between Ryd-
berg states is dominated by the van der Waals interaction \( V_{\text{aw}}(r) = C_6/r^6 \). In the following, we are interested in a repulsive van der Waals interaction \( C_6 > 0 \) and red detuning for the two-photon transition \( \Delta < 0 \); the generalization to attractive interactions with blue detuning is straightforward. Then, the weak dressing of the two-ground state atoms gives rise to the induced interaction \( V_{\text{eff}}(r) \sim \Omega^4/16\Delta^2 C_6/r^6 \) at large distances \( r \gg \xi_0 \equiv (C_6/(2\hbar|\Delta|))^{1/6} \). On the other hand, for short distances \( r < \xi_0 \), the two atoms enter the van-der Waals blocked regime, where only one atom is dressed with the Rydberg state, and the interaction saturates at an energy shift \( \sim \Omega^4/\Delta^2 C_6/\xi_0^6 \). The full interaction potential \( V_{\text{eff}} \) is derived within the adiabatic Born-Oppenheimer approach \( V_{\text{aw}}(r) = \hbar \Omega^4/(|\Delta|^3[1 + (r/\xi_0)^6]^{-1}) \) \([10,11]\), which in Fourier space reduces to

\[
V_{\text{eff}}(q) = \left( \frac{\pi^2}{12} \frac{\hbar \Omega^4}{|\Delta|^3} \right) f(\xi_0 q)
\]  

(1)

with \( f(z) = e^{-z^2} \left[ e^{-z^2/2} - 2 \cos(\sqrt{2}z/2 + \pi/3) \right] /z \). Within first Born approximation, this two-body interaction gives rise to the s-wave scattering length

\[
g_{\text{eff}} = \frac{4\pi \hbar^2 a_{\text{eff}}}{m} = \frac{\pi^2 \hbar \Omega^4}{12 |\Delta|^2 \xi_0^3}.
\]

(2)

Note, that on short distances, additional crossings with the surrounding Rydberg levels appear, which give rise to very narrow resonances and opens up an additional loss channel. However, due to the extremely narrow structure of these resonances one can expect that the particles mainly move diabatically across, and these losses are strongly suppressed; a detailed theoretical analysis of these losses is so far missing.

In the many-body system, the effective interaction between the particles can in general also contain many-body interaction terms. For weak Rydberg dressing with \( (\Omega/\Delta)^2 \ll 1 \), these additional terms become relevant at high particle densities \( n \): first, the two-particle blockade radius \( \xi_0 \) gives rise to a maximal density of excited Rydberg atoms \( 1/\xi_0^3 \) above which collective phenomena become relevant. On the other hand, the density of excited Rydberg atoms due to the weak dressing is given by \( (\Omega/2\Delta)^2 n \). Consequently, the validity of the two-body interaction \( V_{\text{eff}}(r) \) is limited to the dilute regime

\[
n_0^{\text{3}} \ll \frac{4 \Delta^2}{\Omega^2},
\]

(3)

At higher densities \( n \gtrsim n_c = 4|\Delta|^{5/2}/(\Omega^2 \sqrt{C_6}/2) \) a crossover into the collective regime takes place (see dashed line in Fig.1) and the effective interaction is dominated by collective many-body interactions. The behavior \( |\Delta|^5 \sim (C_6 \hbar^2 \Omega^4) \) of this cross-over line derived within this simple estimate agrees with the one expected from the universal scaling theory \([12,19]\).

In the following, we provide a description of this effective interaction for a Bose-Einstein condensate. The idea is to derive for a fixed atomic density \( n \) the internal energy \( E_{\text{eff}}[n] \) of the driven Rydberg system within a Born-Oppenheimer approximation. This internal energy then describes the collective interaction potential giving rise to a generalized Gross-Pitaevskii equation

\[
\imath \hbar \partial_t \psi(t, r) = \{ H_0 + g_n(t, r) + E_{\text{eff}}[n(t, r)] \} \psi(t, r) \]  

(4)

with the condensate wave function \( \psi(t, r) \), the density \( n(t, r) = |\psi(t, r)|^2 \), and the derivative \( E_{\text{eff}}[n] = \partial_n E_{\text{eff}}[n] \). Here, \( H_0 = -\hbar^2 \Delta/(2m) + V_{\text{aw}}(r) - \mu \) describes the non-interacting part with \( V_{\text{aw}}(r) \) the external trapping potential, \( m \) the mass of the particles, and \( \mu \) the chemical potential, while \( g_n \) accounts for the s-wave scattering between ground state atoms. This approach remains valid for momenta of the wave function smaller than the characteristic length scale for the effective interaction.

The internal energy \( E_{\text{eff}}[n] \) can be derived within a mean-field/variational approach. The Hamiltonian for the internal degree of freedom is described by a spin Hamiltonian \([10]\)

\[
H = \sum_i \left( -\frac{\hbar \Delta}{2} \sigma_z^{(i)} + \hbar \Omega \frac{1}{2} \sigma_z^{(i)} + \frac{C_6}{2} \sum_{i \neq j} \frac{P(i) P(j)}{|r_i - r_j|^6} \right),
\]

with \( P(i) = (1 + \sigma_z^{(i)})/2 \) the projection onto the excited Rydberg state \( |r \rangle \). The strong repulsion between the Rydberg atoms gives rise to the correlation function \( g(r_i - r_j) = (P(i) P(j))/f^2 \). The correlation function vanishes on short distances, i.e., \( g(r) \approx 0 \) for \( |r| \ll \xi \), due to the Blockade of Rydberg excitations, and approaches unity \( g(r) \to 1 \) at large distances \( |r| \gg \xi \). The characteristic correlation length scale \( \xi \) denotes the collective blockade radius. Note, that this correlation function is independent on the remaining particle positions due to the homogeneous distribution of the particles in the BEC. A variational wave function, which allows one to include the strong correlations takes the form

\[
|0\rangle = \frac{1}{N} \sum_{s_1 \ldots s_N} \left[ \prod_{i \neq j} C_{s_i s_j} (r_i - r_j) \right] |s_1 \ldots s_N\rangle,
\]

(5)

where \( C_{s s'}(r) \) with \( s \in \{g, r\} \) account for correlations on distances shorter than a characteristic length scale \( \xi \), and reduce to \( C_{s s'} \to \alpha_s \alpha_{s'} \) for large distances with \( \alpha_g = \cos \theta \) and \( \alpha_r = \sin \theta \). Then, this wave function describes a paramagnetic phase with the spins aligned along the direction \( \langle \sigma^{(i)} \rangle \), i.e., \( \cos 2\theta = -\langle \sigma_z^{(i)} \rangle \) and \( \sin 2\theta = -\langle \sigma_z^{(i)} \rangle \), and the fraction of excited Rydberg atoms reduces to \( f \equiv \langle P(i) \rangle = \sin^2 \theta \). Note, that the relation between \( C_{s s'}(r) \) and the correlation function \( g(r) \) is highly non-trivial. In the following, we are interested in using the correlation length \( \xi \) as a variational parameter, and therefore, the precise shape of \( C_{s s'} \) is irrelevant.
The energy density $\epsilon_{\text{var}}(\theta, \xi) = \langle 0 | H | 0 \rangle$ for the internal degree of freedom reduces to

$$\epsilon_{\text{var}}(\theta, \xi) = \frac{\hbar \Delta n}{2} \cos 2\theta - \frac{\hbar \Delta n}{2} \sin 2\theta + \lambda \sin^4 \theta C_6 n^2 \frac{\xi^3}{\xi^3}. \quad (6)$$

The variational parameters are the excited Rydberg fraction $f = \sin^2 \theta$ and the correlation length $\xi$. The dimensionless parameter $\lambda/\xi^3 = \int d^3x g(x)/|x|^6 = 1/\xi^3$. $\int d^3x g(x)/|x|^6$ is determined by the details of the correlation function. It is important to note, that the qualitative behavior of the energy functional is independent on the precise value of $\lambda$, and therefore, this parameter will be fixed by the constraint to reproduce the correct asymptotical behavior at low densities. The dressing of the ground state atoms with the excited Rydberg level leads to an energy shift $\epsilon_0 = -\hbar n \sqrt{\Delta^2 + \Omega^2}/2$ even in absence of Rydberg interactions. Subtracting this contribution, the energy functional $E_{\text{eff}}[n]$, describing the Rydberg dressed interactions in the collective regime, is obtained by the energy for the state adiabatically connected to the non-interacting system: this wave function is obtained by minimizing the energy functional $\epsilon_{\text{var}}$, i.e.,

$$E_{\text{eff}}[n] = \min_{\{v_0\}} [\epsilon_{\text{var}}(\theta, \xi)] - \epsilon_0, \quad (7)$$

for fixed ground state density $n$, Rabi frequency $\Omega$, and detuning $\Delta$. The value $\theta$ for the minimal energy density follows from the equation $\partial_{\theta} \epsilon_{\text{var}}(\theta, \xi) = 0$; note, that this condition is equivalent to the self-consistency equation derived in Ref. $[18]$. On the other hand, the last term in equation (6) always gives a positive contribution to the energy functional, and it will be minimized by maximizing the correlation length $\xi$. However, the correlation length satisfies several constraints: in the weakly interacting regime the correlations due to the Rydberg excitations are limited by the two-particle blockade radius $\xi_0$ $[16]$. Entering the collective regime the distance between the Rydberg atoms is further reduced and the correlations are bounded by $\frac{1}{n_f} \frac{1}{3}$, i.e. $\xi \approx \frac{1}{n_f} \frac{1}{3}$, see inset in Fig. 2. Note, that the qualitative behavior of the system is independent on the precise choice of $\xi$ but only weakly renormalized the dimensionless parameter $\lambda$.

The energy functional $E_{\text{eff}}[n]$ is shown in Fig. 2, for varying density $n$. In the low density regime, $n \ll n_c = 4(\Delta^2/\Omega^2 \sqrt{C_6}/2)$, it reduces to a pure two-particle interaction $E_{\text{eff}} = g_{\text{at}} n^2/2$. The comparison with the exact two-body interaction Eq. (4) allows us to fix the dimensionless parameter $\lambda$ and within first Born approximation it takes the form $\lambda = 2\pi^2/3$. Strong deviation from the two-body interaction can already be seen at densities as low as 0.05$n_c$, see Fig. 2. Collective blockade phenomena give rise to a very broad crossover, with the energy functional $E_{\text{eff}}[n]$ eventually saturating at a chemical potential $E_{\text{eff}}[n] \approx n \mu_{\text{sat}} = nh \left( \sqrt{\Delta^2 + \Omega^2} - |\Delta| \right)/2$ at high densities $n \gg n_c$. This behavior can be understood from the following argument: (i) each atom within a Blockade radius gives rise to an energy shift in the functional, and (ii) in the high density limit to fraction of excited Rydberg atoms vanishes. Therefore, all atoms up to a non-extensive part are within a Blockade radius, and thus basically free.

Finally, we can derive the ground state wave function for a Bose–Einstein condensate in a harmonic trap with the influence of the Rydberg dressed interaction within the Thomas-Fermi approximation. The density profile for the collective many-body interaction is shown in Fig. 2(b) for increasing particle number $N$. A characteristic feature is the strong increase of the density in the trap center. This behavior is a consequence of the linear behavior of the collective interaction potential at high particle densities $n \gg n_c$, and allows one to distinguish the collective interaction from a two-body interaction or heating effects. The density profile for an atomic condensate of $^{87}$Rb atoms with a background scattering length $a_s = 5.7$nm and fixed particle number $N = 10^5$ is shown in Fig. 3. For weak Rydberg dressed interactions, the density profile is given by the inverted parabola profile $n(r) = \left[ \mu - V_{\text{ext}}(r) \right]/g_{\text{off}}$. The crossover into the collective interaction regime is again signaled by the characteristic change in the shape of the atomic cloud.

The total decay rate $\gamma_{\text{eff}}$ for spontaneous emission is given by

$$\gamma_{\text{eff}} = \frac{\Omega_p^2}{4\Delta_p^2} \left( \gamma_r + \frac{\Omega_p^2}{4\Delta_p^2} \right). \quad (8)$$
The detuning $\Delta_p$ and Rabi frequency $\Omega_p$ of the laser coupling the ground state and the intermediate $p$-level only determine the global life time via its ratio $(\Omega_p/\Delta_r)^2$. Second, the Rabi frequency $\Omega_r$ for the coupling to the Rydberg state is limited by experimental restrictions on available laser power. Consequently, the strongest influence of the Rydberg dressed interaction is obtained by the choice of the detuning $\Delta$, which extremizes the induced $s$-wave scattering length for fixed life time of the system, i.e., $\partial g_{eff}/\partial \Delta = 0$. Then, the optimal detuning satisfies $\Delta_c = -[\Omega_r/\gamma_r/(28\gamma_p)]$ with the induced $s$-wave scattering length

$$a_{eff} = \frac{m}{4\pi\hbar^2} g_{eff}(\Delta_c) = \frac{m}{4\pi\hbar^2} \frac{49\pi^2}{48} \sqrt{\frac{C_6}{\gamma^2}} \left(\frac{\Omega_r^2\gamma_r}{28\gamma_p}\right)^{1/4}.$$ 

For $^{87}$Rb weakly dressed with the Rydberg level $|35s\rangle$, the van der Waals interaction takes the strength $C_6 = 1.31\times10^{13}$a.u. [13], and the decay rates $\gamma_r = 4$kHz and $\gamma_p = 6$MHz. For a realistic experimental setup, Rabi frequencies with $\Omega_r = 22$MHz have been reached. Finally, a life time of $\gamma = 6$Hz is sufficient for a fast experiment, and we obtain

$$a_{eff} = 1.36\gamma^2 \text{nmHz}^{-2} = 49.5\text{nm},$$

compared to $a_s = 5.7$nm, which is an increase of the scattering length by an order of magnitude. The optimal detuning reduces to $|\Delta_c| = 107$kHz with the characteristic length scale $\xi_0 = 3\mu$m. The coupling to the $p$-level requires the strength $|\Omega_p/\Delta_p| = \sqrt{\gamma/2\gamma_p} = 7.0\times10^{-4}$, and the effective Rabi frequency becomes $\Omega = 7.8$kHz, thus $|\Omega/\Delta_c| = \sqrt{\gamma/2\gamma_r} = 0.072$. The critical density for the crossover from the two-body interaction to the collective many-body interaction reduces to $n_c = 2.57\times10^{13}$cm$^{-3}$, and consequently, for typical peak densities $n_{\text{peak}} \sim 10^{14}$cm$^{-3}$ of a typical BEC experiment the system is well within the collective regime, and allows for the detection of this novel interaction. Note, that within the collective regime, the number of excited Rydberg atoms is further reduced due to the Blockade phenomena. This in principle allows one to further reduce the detuning without increasing the losses from spontaneous emission. However, in a trapped system, this will increase the losses at the edge of the condensate, where the density drops below the critical density $n_c$.

Finally, we would like to point out, that the weakly dressed Rydberg interaction could be further tuned by a micro-wave field coupling different Rydberg levels [21]. As opposed to the much stronger van der Waals repulsion between the Rydberg levels, the micro-wave field only gives rise to a weak dipole-dipole interaction, which becomes relevant on large distances $r \gg \xi$ due to its slow decay. As a consequence, it does not change the behavior on distances comparable to the Blockade radius. Such a scenario is in analogy to the possibility to tune interaction potentials with cold polar molecules [21], and will allow one to explore the interesting properties of anisotropic dipole-dipole interactions in the collective regime.

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