Diagnosing a two-body state of ultracold atoms with light

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Abstract – An absorption of a weak pulse by two identical atoms moving in a trap is investigated. Based on atom-light interactions we present a microscopic model of a two-body wave function diagnosis. We study the influence of pulse properties on the results. We show that a pulse duration impacts the resulting one-photon and two-photons absorption probabilities significantly.

Introduction. – The enormous development in the field of ultracold atoms in the last 20 years is not only due to the advanced cooling methods [1–3], but also to the imaging techniques. A diagnosis of a Bose-Einstein condensate is always based on atom-light interactions. The multitude of possibilities created by this phenomenon allows researchers to deeply examine various aspects of quantum systems at extremely low temperatures [4–7].

One of the most widespread experimental methods of investigation of ultracold gases is the absorption imaging. The key role in this technique is played by the fact that the absorption rate is proportional to the column density of atoms, or so it is tacitly assumed. Sending a resonant probe light pulse through a sample and observing the “shadow” left by the atomic absorption with a CCD camera opens access to many relevant properties like the density profiles of atomic clouds and higher-order correlation functions [8–12]. Recently it was even possible to image a single atom [13]. Typically a weak pulse is used to avoid multiple scatterings and therefore enhance the control over the measurement.

Although the general principles of absorption imaging are well understood, there remain some open questions waiting to be addressed. Recently a process of splitting of the Bose-Einstein condensate was analysed [14]. Within the classical field approximation, see for instance [15,16], it was shown that the statistical properties of the condensate depend on the observation time. Whereas it is possible that these findings are not exactly related to a real quantum measurement with light, the role of the spatial and temporal properties of a light pulse in the absorption imaging, to the best of our knowledge, was not analysed in detail. Well-controlled experiments with just a few trapped atoms are now possible [17,18]. Such a simple system offers the unique opportunity to scrutinize the absorption imaging method at the microscopic level.

To shed more light on this problem we present an oversimplified example of only two atoms located in a spherical harmonic trap. Then, a diagnosis of the system with a light pulse is done through the absorption. Identifying one-photon and a two-photon absorption probabilities as a source of a one-particle density distribution and two-body distribution, respectively, we study the influence of pulse properties on the results.

Model. – Our method of diagnosing the two-body wave function is based on the absorption of sufficiently well-collimated light pulses by atoms —both bosons and fermions. The probabilities of one or two photons being absorbed should be measured for different positions of light beams. Out of the estimated likelihoods we may find one-particle density distribution and two-body distribution, respectively, we study the influence of pulse properties on the results.

The total Hamiltonian of the two contact interacting ultracold particles of equal masses \( m_1 = m_2 \) absorbing photons from a light beam reads

\[
H = H_{FS} + H_{AF}. \tag{1}
\]
The term $H_{FS}$ stands for the free system Hamiltonian. It can be written as

$$H_{FS} = \sum_{i=1}^{2} \left( T_i(r_i) + V_i(r_i) \right) + V_f(r_1 - r_2)$$

where $T_i(r_i) = -\hbar^2 \nabla_i^2 r_i$ is the kinetic energy of an atom and $V_i(r_i) = \frac{1}{2} m_i \omega_i^2 r_i^2$ is the harmonic trapping potential. The short-range interaction term for ultracold bosons is expressed by $V_f(r) = g_0 \delta_{ps}(r)$ with $\delta_{ps}(r)$ standing for the pseudo potential which depends on dimensionality, see [19]. The interactions strength $g$ can be either positive or negative. Its dependence on the 3D scattering length for quasi-1D or quasi-2D trap was found in [20,21] and verified experimentally in [22]. Note that for two ultra cold fermions in the same spin state $V_f(r) = 0$. We denote the spatial part of $H_{FS}$ as $H_S$. The last sum in eq. (2) describes the internal structure of atoms, which is in a form of a simple two-level model [23]. Here $\{g\}$ indicates the ground state, $\{e\}$ stands for the excited state and $\hbar \omega_0$ is the energy difference between two states.

The interaction of atoms with a beam is represented by the $H_{AF}$ term:

$$H_{AF} = \hbar \lambda \sum_{i=1}^{2} \left( \sigma^+_i + \sigma^-_i \right)$$

$$\times \left( \epsilon(r_i, t) e^{i(k_L \cdot r_i - \omega_L t)} + \text{c.c.} \right)$$

$$\approx \hbar \lambda \sum_{i=1}^{2} \left( \sigma^+_i e^{i(k_L \cdot r_i - \omega_L t)} + \sigma^-_i e^{-i(k_L \cdot r_i - \omega_L t)} \right),$$

where $\sigma_{\pm}$ are the ladder operators defined as $\sigma_+ = |e\rangle \langle g|$, $\sigma_- = |g\rangle \langle e|$. The expression in the last line of eq. (4) is obtained by using the Rotating-Wave Approximation (RWA) [23]. We assume a weak classical nearly monochromatic beam with an electric field given by $E(r, t) = E_0 (\epsilon(r, t) e^{i(k_L \cdot r - \omega_L t)} + \epsilon^*(r, t) e^{-i(k_L \cdot r - \omega_L t)})$, where $E_0$ indicates a real-valued magnitude of an amplitude of the electric field, $k_L$ a wave vector and $\omega_L$ an angular frequency of the light. An envelope of a light pulse denoted by $\epsilon(r, t)$ is spatially and temporally dependent. We assume a weak intensity of the pulse so that the parameter $\lambda = \frac{E_0}{\hbar \omega_0}$ is small as compared to the other terms in the total Hamiltonian. Here $d$ stands for the transition dipole moment of the atom.

A state vector $\Psi(r_1, r_2, t)$ of two atoms within our model can be written in a general form as

$$\Psi(r_1, r_2, t) = \left( \begin{array}{c} \phi(r_1, r_2, t) |gg\rangle \\ \frac{1}{\sqrt{2}} (\chi_1(r_1, r_2, t) |eg\rangle \pm \chi_2(r_1, r_2, t) |ge\rangle) \\ \eta(r_1, r_2, t) |ee\rangle \end{array} \right)$$

where the $+$ sign on the second line of the state vector corresponds to bosons, whereas the $-$ sign to fermions.

The time-dependent Shrödinger equation $i \hbar \frac{d \Psi}{d t} = H \Psi$ can be expressed as a system of equations for unknown functions $\phi, \chi_1, \chi_2$ and $\eta$ by

$$i \hbar \dot{\phi} = (H_S - \hbar \omega_0) \phi + \frac{\hbar \lambda}{\sqrt{2}} \left( \epsilon^*(r_1, t) e^{-i(k_L \cdot r_1 - \omega_L t)} \chi_1 \\
\pm \epsilon^*(r_2, t) e^{-i(k_L \cdot r_2 - \omega_L t)} \chi_2 \right),$$

$$i \hbar \dot{\chi}_1 = H_{S\chi_1} \pm \sqrt{2} \hbar \lambda \left( \epsilon(r_1, t) e^{i(k_L \cdot r_1 - \omega_L t)} \phi \\
+ \epsilon^*(r_2, t) e^{-i(k_L \cdot r_2 - \omega_L t)} \eta \right),$$

$$i \hbar \dot{\chi}_2 = H_{S\chi_2} \pm \sqrt{2} \hbar \lambda \left( \epsilon(r_2, t) e^{i(k_L \cdot r_2 - \omega_L t)} \phi \\
+ \epsilon^*(r_1, t) e^{-i(k_L \cdot r_1 - \omega_L t)} \eta \right),$$

$$i \hbar \dot{\eta} = (H_S + \hbar \omega_0) \eta + \frac{\hbar \lambda}{\sqrt{2}} \left( \epsilon(r_1, t) e^{i(k_L \cdot r_1 - \omega_L t)} \chi_1 \\
\pm \epsilon(r_2, t) e^{i(k_L \cdot r_2 - \omega_L t)} \chi_2 \right).$$

The above system of equations may be solved approximately in the following way. As was mentioned before we consider a very weak driving to neglect the depletion of the initial state. We also assume that initially the two atoms are in the internal ground states, namely that for $t = 0$ the state vector $\Psi(r_1, r_2, 0) = \phi(r_1, r_2, 0) |gg\rangle$. Therefore we assume that during the interaction between the system and the light the state vector remains almost unchanged, that is to say $|\phi| \gg |\chi_1|, |\chi_2| \gg |\eta|$ for the duration of the pulse. Then, introducing the interaction picture by the following substitutions $\phi \rightarrow e^{i \omega_0 t} \phi, \eta \rightarrow e^{-i \omega_0 t} \eta$ and $\chi_1(2) \rightarrow e^{-i H_{S\chi}/\hbar} \chi_1(2)$, we obtain the final equations

$$\phi = e^{-i H_{S\chi}/\hbar} \phi(r_1, r_2, 0),$$

$$\dot{\chi}_1 = -i \sqrt{2} \lambda e^{i H_{S\chi}/\hbar} \epsilon(r_1, t) e^{i k_L \cdot r_1 - i \Delta t} \phi,$$

$$\dot{\chi}_2 = +i \sqrt{2} \lambda e^{i H_{S\chi}/\hbar} \epsilon(r_2, t) e^{i k_L \cdot r_2 - i \Delta t} \phi,$$

$$\dot{\eta} = -i \frac{1}{\sqrt{2}} \lambda (e^{i H_{S\chi}/\hbar} \epsilon(r_2, t) e^{i k_L \cdot r_2 - i \Delta t} \chi_1$$

$$+ e^{i H_{S\chi}/\hbar} \epsilon(r_1, t) e^{i k_L \cdot r_1 - i \Delta t} \chi_2),$$

where we define a detuning by $\Delta = \omega_L - \omega_0$. As we may note the final form of the above system of equations comes directly from the fact that in the general case $e^{i k_L \cdot r(t)} e^{i H_{S\chi}/\hbar} H_S \neq 0$.

**Solutions.** – The analytical solutions of the spatial Hamiltonian $H_S$ are well known both for two ideal bosons or fermions ($V_f(r) = 0$) and for two interacting ultra cold bosons [19]. We assume a rectangle pulse envelope. When the light is on $\epsilon(r, t) = \epsilon(r)$. Thus it is possible to solve eq. (6) analytically. Without loss of generality we choose the initial state as an eigenvector of $H_S$, namely $\phi(r_1, r_2, 0) = \phi_0(r_1, r_2)$ with the index $n$ indicating the
$n$-th eigenvector in a chosen basis. Then, using Dirac notation and the formula $e^{-iE_n t/\hbar} = \sum e^{-iE_i t/\hbar} \langle \phi_i | \phi \rangle$ with $E_i$ standing for the $i$-th eigenvalue, we find the general solution for $\chi_1$, $\chi_2$ and $\eta$ as

$$\phi = e^{-iE_n t/\hbar} | \phi_n \rangle,$$

$$\chi_1 = -\sqrt{2} \sum_i \epsilon_{in} \left( \frac{e^{i\Delta_{in} t} - 1}{\Delta_{in}} + \frac{e^{i\Delta_{in} t} + 1}{\Delta_{in}} \right) | \phi \rangle,$$

$$\chi_2 = \mp \sqrt{2} \sum_i \epsilon_{in} \left( \frac{e^{i\Delta_{in} t} - 1}{\Delta_{in}} - \frac{e^{i\Delta_{in} t} - 1}{\Delta_{in} + \Delta_{kn}} \right) | \phi \rangle,$$

$$\eta = -\lambda^2 \sum_{i,k} \epsilon_{ik} \frac{\Delta_{kn}}{\Delta_{ik} + \Delta_{kn}} \left( \epsilon_{ik} e_{ik} - \epsilon_{ik} e_{ik} \right) \left( 1 + e^{i\Delta_{ik} t} \right) \left( 1 - e^{-i\Delta_{ik} t} \right) | \phi \rangle,$$

where $\epsilon_{ij} = \langle \phi_i | e^{i\mathbf{k}\cdot\mathbf{r}} | \phi_j \rangle$, $\epsilon_{ij} = \langle \phi_i | e^{i\mathbf{k}\cdot\mathbf{r}} | \phi_j \rangle$ and obviously $\epsilon_{ij} = \epsilon_{ji}$. Here we define the scalar product by $\langle \phi_i | \phi_j \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_i^*(\mathbf{r}_1, \mathbf{r}_2) \phi_j(\mathbf{r}_1, \mathbf{r}_2)$. The generalized energy difference between the $i$-th and $j$-th states reads $\Delta_{ij} = \Delta_{ij} - \Delta = E_{ij} - \epsilon_{ii} - \Delta$. Note that for resonant terms, i.e., $\Delta_{ij} = 0$ in any sum of eq. (7) the proper element has to be evaluated by taking the limit $\Delta_{ij} \to 0$.

The resonant term behaves as $t$ for $\chi_1$, $\chi_2$ and as $t^2$ for $\eta$. For the clarity of our argumentation hereafter we will take the resonant case with $\Delta = 0$, but our conclusions will hold also for $\Delta \neq 0$.

The probabilities of having one or two photons absorbed by atoms are easily defined by $P_1(t) = |\chi_1|^2 + x_2 |\chi_2|^2 = |\chi_1|^2 + |\chi_2|^2$ and $P_2(t) = |\eta|^2 = |\eta|^2$. After some straightforward calculations they can be expressed as

$$P_1(t) = 2\lambda^2 |\epsilon_{nn}|^4 t^2 + 4\lambda^2 \sum_{\substack{i \neq n \\kappa \neq \kappa'}} |\epsilon_{i\kappa n}|^2 \left( 1 - \cos(\Delta_{in} t) \right),$$

$$P_2(t) = \lambda^4 |\epsilon_{nn}|^4 t^4 + 4\lambda^4 \sum_{\substack{i \neq n \\kappa \neq \kappa'}} |\epsilon_{ik\kappa n}^*| \epsilon_{ik\kappa n} \epsilon_{ik\kappa n} \rho_{i\kappa\kappa'} n |i\kappa'\kappa'\kappa n|.$$

where $\rho_{i\kappa\kappa'}(n)$ is of order $o(t^4)$. Its definition can be found in the footnote $^1$. A short-time characteristic of the probabilities, when $t \ll \Delta_{in}^{-1}$ with $i$ corresponding to the nearest eigenvalue to $n$, reads

$$P_1(t) \approx 2\lambda^2 |\epsilon_{nn}|^2 (e^{i\mathbf{r}_1 \cdot \mathbf{r}_1})^2, \quad t \to 0,$$

$$P_2(t) \approx \lambda^4 |\epsilon_{nn}|^4 (e^{i\mathbf{r}_2 \cdot \mathbf{r}_2})^2 |\phi_n|^2 t^4, \quad t \to 0.$$

The analysis of eqs. (8), (9), (11) and (12) reveals an intriguing discrepancy between the short-time and the long-time behaviour of the probabilities. First of all, the long-time probabilities depend on the couplings between an actual state of the system and different eigenstates that occur because, for the experimental relevance, the beam width must be narrower than the characteristic system width. This fact automatically leads to the conclusion that for longer pulses the information about the actual state of the system is blurred. Secondly, although the dominant terms are of the same order in both situations, the coefficients determining their magnitude are not. For the short time the probabilities coefficients are related to the intensity $|\epsilon(\mathbf{r})|^2$. Note that for $P_1(t), t \to 0$ the coefficient in front of $t^2$ can be rewritten as $/\phi_n'(x) e^{i\mathbf{k}_{x}}$ with the one-particle density $\rho(\mathbf{r}) = \int d\mathbf{r}_n' |\phi_n(\mathbf{r}, \mathbf{r}_n')|^2$, which is a very intuitive result. On the other hand the coefficients for the long time depends on the amplitude of the pulse proportional to $|\epsilon(\mathbf{r})| e^{i\mathbf{k}_{x}}$ rather than to its intensity alone.

In the next section we are going to show the most striking examples of the above differences.

Results. — In this section we present the results obtained with our model which are mimicking an experiment diagnosing a quantum state of two ultra-cold atoms. We restrict our findings to a quasi-1D system which captures all essentials features of our model and provides with a clear picture. In a real experiment it corresponds to cigar-shaped traps with a very strong transverse confinement. We send a probing light pulses along the transverse direction $z$ which is related to an electric field $\mathbf{E}(\mathbf{r}, t) = E_0(\epsilon(x) e^{i(k_x z + \omega_L t)} + \epsilon^*(x) e^{-i(k_x z + \omega_L t)})$ with $k_L = |k_L|$. We may also assume that $1/k_L$ is much bigger than the typical transverse length of a probe, so that the driving term $e^{\pm i(k_L \mathbf{z})}$ may be neglected. As the initial state $\phi(x_1, x_2, 0)$ we select the ground state both for ideal fermions or bosons and interacting bosons.

One-particle density function. In order to find a one-particle density function we use a single pulse with $|\epsilon(x) x_0, \sigma \rangle = \frac{1}{\sqrt{\sigma}} e^{-(x-x_0)^2/\sigma^2}$. Then, using the short-time characteristic of $P_1(t)$ expressed by eq. (11) we evaluate the probability of one-photon absorption as a function of the position of the pulse center $x_0$. We compile our results for two ideal or interacting bosons and two fermions in fig. 1. As we may note by comparing with the well-known analytical solutions of $H_S$ for the ground state the one-photon absorption diagnosis gives a direct access to the one-particle density distribution $\rho(x)$ defined in the preceding section. A clear difference between the interacting and non-interacting case is seen as well as between bosons and fermions. The repulsive system distribution
is wider than that of an ideal gas, while the attractive system one is narrower than that of an ideal gas. 

The analysis of eq. (8) shows that using a pulse that is too long may affect the measured one-particle density profile. For pulses with complicated wave fronts the coefficients in the eq. (8) would differ significantly from those of eq. (11). To illustrate the unwanted field amplitude dependence of the result for long pulses we choose the extreme example of a pulse with cross-section given by 

$$e(x; x_0, \sigma) = \frac{1}{\sigma \sqrt{\pi}} e^{-(x-x_0)^2/\sigma^2} \text{sgn}(x),$$

with \(\text{sgn}(x)\) staying |\(\phi_G\)\rangle staying the ground state of \(H_S\). Here we neglect interference terms like \(\epsilon(x-x_1)^2/\sigma^2 \epsilon(x-x_2)^2/\sigma^2\), that in experiment can be realized either by ensuring \(|x_1 - x_2| > 3\sigma\) or by introducing a phase difference between the two pulses and averaging over many measurements. The last two terms of a sum in the above equation are corresponding to processes where two photons were absorbed at the same space point. The probability of such a process should be measured independently and then subtracted from the total result of the two-photon absorption.

The easiest way to notice that is by the assumption that \(|\epsilon(x; x_1, \sigma)|^2 \approx \delta(x - x_1)\), which makes \(\langle \phi_G | |\epsilon(x; x_1, x_2, \sigma)|^2 |\epsilon(y; x_1, x_2, \sigma)|^2 \langle \phi_G \rangle \approx 2 |\phi_G(x_1, x_2)|^2 + |\phi_G(x_1, x_1)|^2 + |\phi_G(x_2, x_2)|^2\).

We sum up our considerations with an example of two repulsive bosons with interaction strength \(g = 6\). The total two-photon absorption probability \(P_2(t)\) was found for \(t_0 = 0.0001 \Delta_{10}^{-1}\) and for several beam positions \(x_1\) and \(x_2\). Then we subtract from it the probabilities of a single pulse two-photon absorption. Finally we compare our findings with the analytical solution for \(\phi_G(x, y)\) which is plotted in fig. 3. It is a straightforward observation that we reconstructed the actual two-body wave function density with our model.

Analogously to the previous subsection the results for a long pulse in the time domain when eq. (9) holds may lead to a wrong two-body wave function. One more time we use the example of the highly modified wave front with 

$$e(x; x_1, x_2, \sigma) = \frac{1}{\sigma \sqrt{\pi}} e^{-(x-x_1)^2/\sigma^2 + (x-x_2)^2/\sigma^2} \text{sgn}(x).$$

The resulting two-photon probability absorption \(P_2(t)/4t^4\) for \(t_0 = 0.0001 \Delta_{10}^{-1}\) and \(t = \Delta_{10}^{-1}\) for two interacting bosons with \(g = 6\) as a function of beam positions can be found in fig. 4. For the result based on eq. (9) we truncate the sum at \(i = 20\) ensuring that adding another eigenstate would not change the result up to 1% accuracy. We find that...
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**Fig. 3:** (Colour online) Two-photon absorption probability $P_2(x_1, x_2; t_0, \sigma)/\lambda^4 t_0^4$ for two interacting bosons with $g = 6$ as a function of beam positions $x_1$ and $x_2$ for $t_0 = 0.0001\Delta^{-1}$ after subtracting a single beam two-photon absorption (right). The oscillatory units are used. The left plot shows the analytical solution of $|\phi_G(x_1, x_2)|^2$ for $g = 6$.

**Fig. 4:** (Colour online) Two-photon absorption probability $P_2(x_1, x_2; t_0, \sigma)/\lambda^4 t_0^4$ for two interacting bosons with $g = 6$ as a function of beam positions $x_1$ and $x_2$ for $t_0 = 0.0001\Delta^{-1}$ (left) and $t_0 = \Delta^{-1}$ (right) after subtracting the single-beam two-photon absorption. The oscillatory units are used.

stress the fact that the pulse duration in an experimental diagnosis should be chosen very carefully.

**Conclusions.** – In conclusions, we studied a simple model of diagnosing a two-body state with light for interacting or ideal bosons and fermions. We demonstrated that the results of an experiment based on our theory would crucially depend on the pulse duration. For sufficiently short pulses, we estimate with our measurement the actual one-particle density function and the two-body wave function. For longer pulses hypothetical experimental findings would be highly biased. The main reason for that is that the calculated probabilities of one-photon or two-photons absorptions are related to the intensity of the light beam for sufficiently short time, whereas for longer time they depend on the amplitude of the pulse. The structure of eq. (8) and eq. (9) can be understood that the probability of the absorption in a space point is strongly blurred by the free evolution of the initial state. Our results can be generalized to systems containing...
more particles which allows to investigate an experimental procedure of diagnosing higher-order correlation functions from the many-body perspective.

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