Quantum Multimode Model of Elastic Scattering from Bose-Einstein Condensates

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Mean field approximation treats only coherent aspects of the evolution of a Bose-Einstein condensate. However, in many experiments some atoms scatter out of the condensate. We study a semianalytic model of two counterpropagating atomic Gaussian wave packets incorporating the dynamics of incoherent scattering processes. Within the model we can treat processes of the elastic collision of atoms into the initially empty modes, and observe how, with growing occupation, the bosonic enhancement is slowly kicking in. A condition for the bosonic enhancement effect is found in terms of relevant parameters. Scattered atoms form a squeezed state. Not only are we able to calculate the dynamics of mode occupation, but also the full statistics of scattered atoms.

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A remarkably universal tool describing a vast majority of experiments with the Bose-Einstein condensates is the celebrated Gross-Pitaevskii equation (GPE). It describes a coherent evolution of the atomic mean field. In the Hartree interpretation, its time-dependent version assumes that each atom of the system undergoes identical evolution. This is a good assumption since in typical experiments the wave packet of the system contains many thousands of particles in the same state. To use a term borrowed from quantum optics, the time-dependent GPE describes stimulated processes. In some experiments [1], however, there is clear evidence of spontaneous processes. For example, in a collision between two condensates, some atoms from colliding quantum matter droplets would inevitably scatter away from them. This is a loss process, which is not accounted for by the conventional GPE. A description of such phenomena calls for the use of quantum fields instead of c-number wave functions. This is not easy since, in general, field equations are nonlinear. Instead of quantum fields, several groups used classical stochastic fields to imitate quantum initiation of spontaneous processes [2]. At this point it is hard to assess the accuracy of these methods. Solid results so far have been obtained only within perturbation theory [3–5]. It is the purpose of this Letter to present the first exact nonperturbative calculation of collisional losses, valid in the regime of Bose enhancement. Our model assumes spherical nonspreading Gaussians for the colliding wave packets. No doubt it will serve as a benchmark test of the validity of various approximate schemes including classical stochastic fields.

A system of bosons interacting via contact potential is described by the Hamiltonian

$$H = -\int d^3r \hat{\Psi}^\dagger(\mathbf{r},t) \frac{\hbar^2\nabla^2}{2m} \hat{\Psi}(\mathbf{r},t) + \frac{g}{2} \times \int d^3r \hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t), \qquad (1)$$

where $\hat{\Psi}(\mathbf{r},t)$ is a field operator satisfying equal time bosonic commutation relations, m is the atomic mass, and g determines the strength of the interatomic interactions. Since the Hamiltonian (1) is of the fourth order in $\hat{\Psi}$, the Heisenberg equation governing the evolution of the field will be nonlinear and thus, in general, analytically and numerically untractable. However, for some physical systems, a Bogoliubov approximation can be applied leading to linear Heisenberg equations. The idea underlying this approximation states that for some cases the field operator might be split into two parts ψ and $\hat{\delta}$. The first contribution describes a macroscopically occupied field and, since its fluctuations are usually small, its operator character might be dropped (ψ becomes a c-number wave function satisfying the GPE). The second part $\hat{\delta}$, representing the fluctuations, requires a full quantum mechanical treatment, but as long as we neglect its backreaction on ψ the evolution of $\hat{\delta}$ will be linear.

In this Letter we consider a process of collision of two strongly occupied Bose-Einstein condensates. The initial state of the system consists of two counterpropagating atomic wave packets and the "sea" of unoccupied modes. For such a system the Bogoliubov approximation can be applied. The splitting of the bosonic field is performed in the following manner:

$$\hat{\Psi}(\mathbf{r},t) = \psi_Q(\mathbf{r},t) + \psi_{-Q}(\mathbf{r},t) + \hat{\delta}(\mathbf{r},t), \qquad (2)$$

where the subscript $\pm Q$ denotes the mean momentum of the colliding condensates and $\psi_Q(\mathbf{r},t) + \psi_{-Q}(\mathbf{r},t)$ satisfies the time-dependent GPE. Upon inserting Eq. (2) into the Hamiltonian (1), one obtains a collection of different terms. We keep only those that lead to the creation or annihilation of a pair of particles,

$$H = -\int d^3r\hat{\delta}^\dagger(\mathbf{r},t)\frac{\hbar^2\nabla^2}{2m}\hat{\delta}(\mathbf{r},t) + g\int d^3r\hat{\delta}^\dagger(\mathbf{r},t)\hat{\delta}^\dagger(\mathbf{r},t)\psi_Q(\mathbf{r},t)\psi_{-Q}(\mathbf{r},t) + \text{H.c.} \tag{3}$$

One can argue that such an approximation gives correct results if and only if the kinetic energy associated with the center-of-mass motion is much larger than the interaction energy per particle, $\hbar^2Q^2/(2m) \gg gn$, where n is the average density of the particles in the condensates. Numerical proof of the above statement in the simplest case of two plane matter waves was given in [3]. Since in the case considered below the average momentum of the wave packet $\hbar Q$ is much larger than the width of the wave packet in the momentum space, the above argument applies. This condition is readily fulfilled in current experiments [1,6,7].

In order to further simplify the dynamics we compare three characteristic time scales of the problem. Assuming σ and $N/2$ are the width and the number of atoms in each wave packet, we define collision time, $t_C = (m\sigma)/(\hbar Q)$, linear dispersion time, $t_{\rm LD} = m\sigma^2/\hbar$ [8], characteristic time of the spread of the wave packet due to the kinetic energy term (neglecting the nonlinearity), and nonlinear dispersion time, $t_{\rm ND} = \sqrt{\pi^{3/2}m\sigma^5/gN}$, the time of ballistic expansion in the Thomas-Fermi approximation [9]. The dynamics of our system depend on the relations between these time scales. Hence we introduce dimensionless parameters: $t_{\rm LD}/t_C = \beta$ and $(t_{\rm LD}/t_{\rm ND})^2 = \alpha$. When the number of elastically scattered atoms is small in comparison with the total number of atoms in both wave packets, and both linear and nonlinear dispersion time scales are much longer than the collision time $[(t_{\rm LD}/t_C) = \beta \gg 1$ and $(t_{\rm ND}/t_C)^2 = \beta^2/\alpha \gg 1]$, we can neglect the change of shape of the macroscopically occupied functions $\psi_Q(\mathbf{r},t)$ during the collision. In our model we use spherically symmetric Gaussian wave functions,

$$\psi_{\pm Q}(\mathbf{r},t) = \sqrt{\frac{N}{2\pi^{3/2}\sigma^3}}\exp\left[\pm iQx_1 - \frac{i\hbar tQ^2}{2m}\right] \times \exp\left\{-\frac{1}{2\sigma^2}\left[\left(x_1 \mp \frac{\hbar Qt}{m}\right)^2 + x_2^2 + x_3^2\right]\right\}, \tag{4}$$

where $\mathbf{r} = (x_1, x_2, x_3)$. In the dimensionless units ($t \equiv t/t_C$ and $x_i \equiv x_i/\sigma$, for $i = 1, 2, 3$), the Heisenberg evolution equation of the field operator $\hat{\delta} \equiv \hat{\delta}\exp(i\beta t/2)$ can be obtained upon substituting (4) into (3),

$$i\beta\partial_t\hat{\delta}(\mathbf{r},t) = -\tfrac{1}{2}(\Delta + \beta^2)\hat{\delta}(\mathbf{r},t) + \alpha e^{-r^2-t^2}\hat{\delta}^\dagger(\mathbf{r},t). \tag{5}$$

The above equation has spherical symmetry. Hence, we decompose $\hat{\delta}$ into the basis of spherical harmonics

$$\hat{\delta}(\mathbf{r},t) = \sum_{n,l,m}R_{n,l}(r)Y_{lm}(\theta,\phi)\hat{a}_{n,l,m}(t), \tag{6}$$

where $\hat{a}_{n,l,m}$ are annihilation operators for a particle in the mode described by n, l, m quantum numbers. A good candidate for $R_{n,l}(r)$ is a set of eigenfunctions of a spherically symmetric harmonic oscillator,

$$R_{n,l}(r) = \sqrt{\frac{2n!a_0^{-3}}{\Gamma(l+n+\frac{3}{2})}}\left(\frac{r}{a_0}\right)^l e^{-r^2/2a_0^2}L_n^{l+1/2}\left(\frac{r^2}{a_0^2}\right), \tag{7}$$

where $L_n^{l+1/2}(x)$ is the associated Laguerre polynomial [10] and a_0, a harmonic oscillator length, is an auxiliary free parameter that can be chosen to minimize the computational effort. The evolution of $\hat{a}_{n,l,m}(t)$ is described by

$$i\partial_t\hat{a}_{n,l,m} = \frac{E_{n,l}-\beta^2}{2\beta}\hat{a}_{n,l,m} + D_{n,l}\hat{a}_{n-1,l,m} + D_{n+1,l}\hat{a}_{n+1,l,m} + \frac{\alpha}{\beta}e^{-t^2}\sum_{n'}C_{n,n',l}\hat{a}^\dagger_{n',l,-m} \tag{8}$$

where coefficients $D_{n,l} = \sqrt{n(n+l+1/2)}/(2\beta a_0^2)$, $E_{n,l} = (2n+l+3/2)/a_0^2$, and

$$C_{n,n',l} = \int_0^\infty r^2drR_{n,l}(r)\exp(-r^2)R_{n'l}(r) = \sqrt{\frac{\Gamma(n+l+\frac{3}{2})\Gamma(n'+l+\frac{3}{2})}{\Gamma(l+\frac{3}{2})^2\Gamma(n+1)\Gamma(n'+1)}}(1+a_0^2)^{-l-3/2} \times\left[\frac{a_0^2}{1+a_0^2}\right]^{n+n'}F\left(-n,-n',l+\frac{3}{2},1/a_0^4\right). \tag{9}$$

Here $F(a,b,c,x)$ is a hypergeometric function [10]. Notice that all coupling coefficients are calculated analytically and the $\hat{a}_{n,l,m}$ operators for different l and m are decoupled. Moreover, Eq. (8) do not depend on quantum number m. With all these simplifications the linear system of Eq. (8) can be solved numerically.

The solution of the set of dynamical Eq. (8) for $\hat{a}_{n,l,m}$ contains the full information about the considered quantum system. In particular, we can reconstruct the operator $\hat{\delta}(\mathbf{r},t)$, using decomposition defined in Eq. (6). Since the Hamiltonian (3) is quadratic in $\hat{\delta}$ and the initial state is a vacuum state, than, in the Schrödinger picture, at any later time t the state of scattered atoms is a multimode squeezed state [11].

The most straightforward observable quantity, the number of elastically scattered atoms as a function of time can be expressed in terms of the trace of the density matrix

$$S(t) = \int d^3r\langle\hat{\delta}^\dagger(\mathbf{r},t)\hat{\delta}(\mathbf{r},t)\rangle = \sum_{n=0}^\infty\sum_{l=0}^\infty(2l+1)\langle\hat{a}^\dagger_{n,l,m}(t)\hat{a}_{n,l,m}(t)\rangle, \tag{10}$$

where $(2l+1)$ accounts for the degeneracy of Eq. (8) with regards to the quantum number m [12]. In the limit where

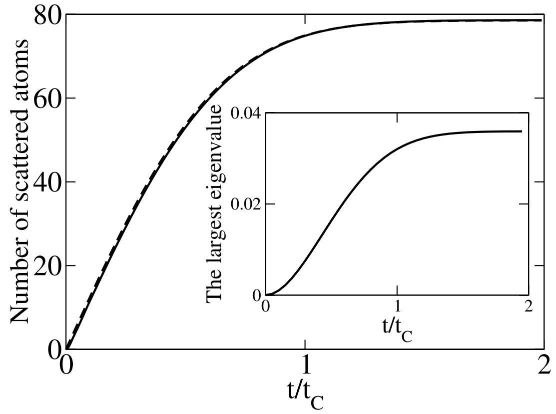

FIG. 1. Number of scattered atoms versus time in perturbative regime. Dashed line: analytical result given by (11). Solid line: numerical result obtained from our model [using Eq. (10)] for $\alpha = 20$ and $\beta = 60$ [16]. The inset shows the time evolution of the largest eigenvalue of the density matrix.

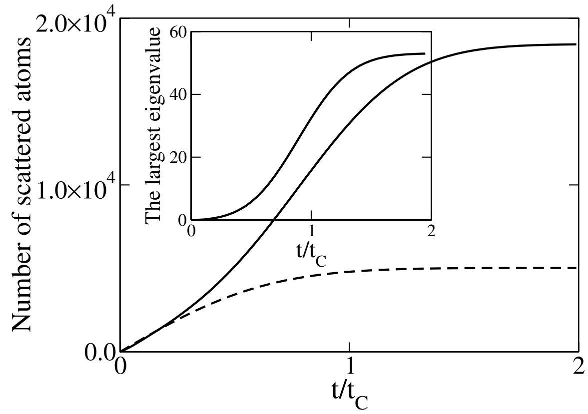

FIG. 2. Number of scattered atoms versus time in nonperturbative regime where the bosonic enhancement occurs. Dashed line: analytical result given by (11). Solid line: numerical result obtained from (10). Parameters are $\alpha = 160$, $\beta = 40$ [16]. The inset shows the time evolution of the biggest eigenvalue of the density matrix.

α/β is small [notice that in Eq. (8), this coefficient multiplies the source term], $S(t)$ can be evaluated in the first order perturbation approximation giving [3]

$$S(t) = \frac{\pi\alpha^2}{16}\mathrm{erf}(\sqrt{2}t). \tag{11}$$

The same result is obtained using imaginary scattering length method [4]. The quality of this approximation is illustrated in Fig. 1.

The bonus of having solved the full set of operator equations is that calculating the full density matrix of the system of scattered atoms $[\rho(\mathbf{r}, \mathbf{r}', t) = \langle \hat{\delta}^\dagger(\mathbf{r}, t)\hat{\delta}(\mathbf{r}', t)\rangle]$ or even higher order correlation functions is just as easy as finding $S(t)$. In the basis (6), due to the decoupling property, density matrix can be written as a direct product of $\rho_{n,n',l,m} = \langle \hat{a}^\dagger_{n,l,m}(t)\hat{a}_{n',l,m}(t)\rangle$ matrices, for different l and m. In the inset of Fig. 1 we present the time evolution of the largest of the eigenvalues of the density matrix $\rho(\mathbf{r}, \mathbf{r}', t)$. Because of the normalization of the density matrix, $\Sigma_i \lambda_i(t) = S(t)$, where λ_i are the eigenvalues of the density matrix, the inset of Fig. 1 shows that for $\alpha = 20$, $\beta = 60$ there is much less than one particle even in the mostly populated eigenmode.

Figure 2 shows analogous comparison between perturbative solution (11) and formula (10) in the regime of parameters where the perturbation theory is expected to fail (the criterion for bosonic enhancement is $\alpha/\beta > 1$, where α/β is proportional to interaction strength g, density of the condensates N/σ^3, and collision time $t_C = m\sigma/\hbar Q$ [13]). The figure shows that, until some critical time, approximately equal to $0.2t_C$, both the perturbative and full solutions agree very well. At this critical time the formula (10) exceeds the perturbative solution and the difference between curves rapidly grows in time. At the same time the biggest eigenvalue of the density matrix of the system reaches one, which means that there is one particle in the mostly populated eigenmode. This observation gives explanation to the growing discrepancy between two curves shown in Fig. 2. Once approximately one atom is scattered into one of the eigenmodes of the density matrix, the probability of scattering another atom into this mode grows rapidly. This is due to bosonic statistics of the scattered atoms and is called the bosonic enhancement effect.

Interesting information about the system might be obtained upon analyzing the largest eigenvalues of $\rho_{n,n',l,m}$ for each quantum number l. Figure 3 juxtaposes these eigenvalues as a function of l, for the case with bosonic enhancement. The plot shows that the density matrix has several eigenvalues of the same order.

From the experimental point of view, coherence properties of the scattered atoms are of great importance. These

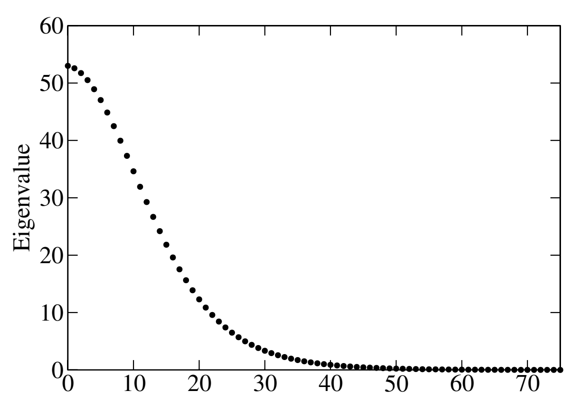

FIG. 3. The biggest eigenvalue of the density matrix for different l for $\alpha = 160$ and $\beta = 40$, at time $t = 2t_C$. The density matrix has several eigenvalues of the same order.

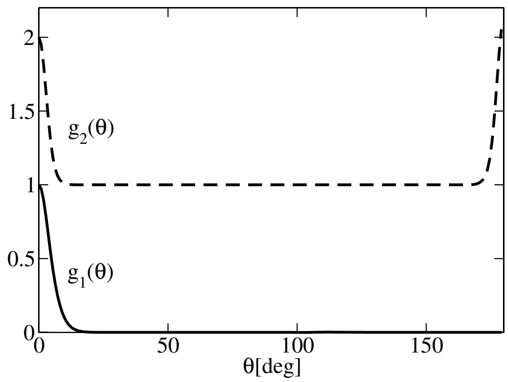

FIG. 4. First and second order correlation functions in momentum space $g_1(\mathbf{k}, \mathbf{k}')$ and $g_2(\mathbf{k}, \mathbf{k}')$ for $|\mathbf{k}| = |\mathbf{k}'| = Q$, as a function of relative azimuthal angle θ at $t = 2t_C$ for $\alpha = 160$, and $\beta = 40$.

properties are best characterized by the correlation functions. In particular, the first and the second order correlation functions can be measured in experiment. In one of the most commonly used methods, time-of-flight measurement, the momentum distribution of the system is obtained. Thus here we calculate the first and the second order correlation functions in momentum space using

$$g_1(\mathbf{k}, \mathbf{k}', t) = \frac{\langle \hat{\delta}^\dagger(\mathbf{k}, t)\hat{\delta}(\mathbf{k}', t)\rangle}{\sqrt{\langle \hat{\delta}^\dagger(\mathbf{k}, t)\hat{\delta}(\mathbf{k}, t)\rangle\langle \hat{\delta}^\dagger(\mathbf{k}', t)\hat{\delta}(\mathbf{k}', t)\rangle}} \quad (12)$$

for the former, and

$$g_2(\mathbf{k}, \mathbf{k}', t) = \frac{\langle \hat{\delta}^\dagger(\mathbf{k}, t)\hat{\delta}^\dagger(\mathbf{k}', t)\hat{\delta}(\mathbf{k}', t)\hat{\delta}(\mathbf{k}, t)\rangle}{\langle \hat{\delta}^\dagger(\mathbf{k}, t)\hat{\delta}(\mathbf{k}, t)\rangle\langle \hat{\delta}^\dagger(\mathbf{k}', t)\hat{\delta}(\mathbf{k}', t)\rangle} \quad (13)$$

for the latter. Because of spherical symmetry of the Heisenberg equation for $\hat{\delta}$, the momentum density $\langle \hat{\delta}^\dagger(\mathbf{k}, t)\hat{\delta}(\mathbf{k}, t)\rangle$ is spherically symmetric as well.

According to Wick theorem and since the anomalous density for $\mathbf{k} = \mathbf{k}'$ is zero $[\langle \delta^\dagger(\mathbf{k}, t)\delta^\dagger(\mathbf{k}, t)\rangle = 0]$, the nth order correlation satisfies a relation $g_n(k, k) = n!$. It is confirmed by numerical results. The solid line in Fig. 4 shows the first order correlation function (12) plotted for fixed length of the $\mathbf{k}$ and $\mathbf{k}'$ vectors ($|\mathbf{k}| = |\mathbf{k}'| = Q$) as a function of relative angle θ. As expected, for $\theta = 0$ the condition, $g_1(\mathbf{k}, \mathbf{k}) = 1$ is satisfied. Also, the limited coherence angle, due to spontaneous initiation of the scattering process, is clearly visible. The dashed line in Fig. 4 shows the second order correlation function (13). Once again, a prediction $g_2(\mathbf{k}, \mathbf{k}) = 2$ is met. As Fig. 4 shows, the g_2 function reveals a strong correlation between atoms scattered in the directions $\mathbf{k}$ and $-\mathbf{k}$, which corresponds to the relative angle $\theta = 180°$. This is an intuitive result, since atoms get scattered in pairs in such a way that the momentum and energy conservation laws are satisfied. Finally, the width of the correlation peak of g_2 in the forward direction in the perturbative regime scales as $1/\beta$, which is proportional to the size of colliding wave packets [13]. This is in analogy to the Hanbury Brown and Twiss method of estimating sizes of distant stars by measuring the intensity-intensity correlation function [14] or relating the density-density correlation of π mesons to the size of the fireball in high energy collision of hadrons [15].

In conclusion, upon analyzing the quantum model of two counterpropagating atomic Gaussian wave packets we get a deeper insight into processes of elastic collision losses of atoms and are able to study the transition from the spontaneous regime to the bosonic enhancement. Scattered atoms form a squeezed state that can be viewed as a multicomponent condensate. Within this model in principle all order correlation functions are accessible and hence it has a high predictive power.

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