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Decay of trapped ultracold alkali atoms by recombination

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Using the knowledge of two-body collision properties that has recently become available, we estimate the three-body recombination rate for doubly-spin-polarized ultracold gas samples of ^{7}Li, ^{23}Na and ^{87}Rb on the basis of the Jastrow approximation. We find that only recombination leading to the formation of the highest two-body bound states is important. The rate for the highest bound level with zero angular momentum is found to increase strongly with the absolute value of the two-body scattering length.

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I. INTRODUCTION

One of the main goals of neutral atom cooling and trapping experiments is achieving the low temperatures and high densities needed to obtain Bose-Einstein condensation (BEC). The past year has shown a rapid growth in phase space density towards or even beyond the critical line of the phase transition by several authors [1–4]. With the recent breakthrough to BEC by Anderson *et al.* [1] it becomes of increasing importance to explore the limits to BEC as imposed by inelastic two-body collisions and by three-body recombination. In this paper we concentrate on the latter process in a cold gas sample of doubly polarized atoms, leading to the formation of triplet ground-state dimers and thus to decay of the atomic density and to heating of the gas. During the last decade much effort has been devoted to calculating the three-body recombination rate constant L for doubly-spin-polarized atomic hydrogen [5–8]. For the alkali atomic species the only published calculation is the estimate in Ref. [9] for Cs. We will now apply the same approximative method to estimate L for cold gas samples of ^{7}Li, ^{23}Na, and ^{87}Rb making use of the recently obtained triplet collision parameters for these alkali-metal atoms [10–13]. The information obtained from an analysis [14] of experimental collisional frequency shifts of the cesium atomic fountain clock is not of sufficient accuracy to enable us to include Cs in our calculations on the same footing as the above-mentioned alkali systems.

An important difference of the alkali-atom recombination process with the previously considered case of atomic hydrogen is the existence of triplet two-body bound states of alkali-metal atoms. This makes recombination possible in three-body collisions without spin flip, enhancing the rate by about ten orders of magnitude [9] with respect to that in H.

This paper is organized as follows. In Sec. II we describe our method of calculation in more detail than in Ref. [9], starting with some general aspects of the three-body recombination process, introducing the Jastrow approximation, and describing the numerical approach. In Sec. III we present our results. A summary and outlook is formulated in Sec. IV.

II. METHOD

A. Rate constant for recombination

We first introduce the notation to be used in the following. Leaving out temporarily the identical-particle aspects, we assume that in a collision of three initially free atoms 1, 2, and 3, particles 2 and 3 form a molecule in the final state, while particle 1 remains free. It is then customary to use Jacobi coordinates $\vec{r},\vec{R}$, where $\vec{r}$ is the radius vector from 2 to 3, and $\vec{R}$ the radius vector from the center of mass of 2 and 3 to 1 (see Fig. 1). The conjugate (Jacobi) momenta are

$$\vec{p}=\frac{1}{2}(\hbar\vec{k}_3-\hbar\vec{k}_2), \tag{1}$$

$$\vec{q}=\frac{2}{3}\hbar\vec{k}_1-\frac{1}{3}(\hbar\vec{k}_2+\hbar\vec{k}_3), \tag{2}$$

where $\hbar\vec{k}_i$ is the momentum of atom i.

We start from a rigorous expression for the transition probability per unit of time for recombination in a three-body collision, assuming normalization in a large six dimensional (6D) volume $\mathscr{V}\times\mathscr{V}$ of the combined $\vec{r}$ and $\vec{R}$ spaces:

$$\omega_{fi}=\sum_{vlm}\sum_{\vec{q}_f}\frac{2\pi}{\hbar}|\langle\phi_f|V(r_{12})+V(r_{13})|\Psi_i^{(+)}\rangle|^2\delta(E_f-E_i). \tag{3}$$

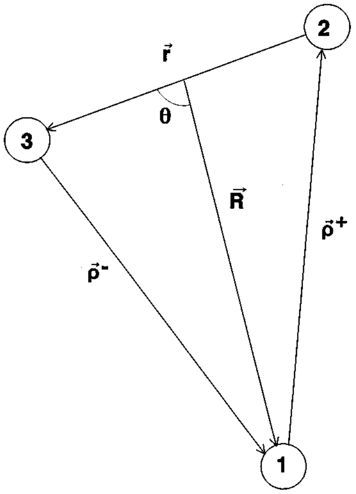

FIG. 1. Coordinates used for three-body scattering. It is assumed that particles 2 and 3 recombine.

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Here $|\phi_f\rangle$ is a stationary state $|\varphi_{vlm}\rangle\otimes|\vec{q}_f\rangle$ of a Hamiltonian H_1 obtained from the total Hamiltonian $H=H_0+V$ by subtracting the interactions of particle 1 with the remaining particles, $|\varphi_{vlm}\rangle$ denoting a particular molecular bound state and $|\vec{q}_f\rangle$ a momentum eigenstate of atom 1 relative to the molecular center of mass. The state $|\Psi_i^{(+)}\rangle\equiv|\Psi_i^{(+)}(\vec{p}_i,\vec{q}_i)\rangle$ is the rigorous three-body eigenstate including the sum V of all interactions, which is asymptotically equal to the free state $|\vec{p}_i,\vec{q}_i\rangle$ of three free atoms supplemented with outgoing scattered parts. For the interaction operator V we will consider only a sum of (triplet) pair interactions,

$$V=V_{12}+V_{13}+V_{23}. \qquad (4)$$

The transition probability (3) is sometimes considered as a rigorous variant of an approximate expression based on Fermi's golden rule, which would contain a continuum eigenstate $|\vec{p}^{(+)},\vec{q}\rangle$ of H_1 as an "unperturbed" state instead of $|\Psi_i^{(+)}\rangle$. Note that we omit the (trivial) electron-nuclear spin parts in our notation.

We now take the limit $\mathscr{V}\rightarrow\infty$ leading to a δ-function normalization of momentum eigenstates. Furthermore, we take care of the identical-particles aspect by replacing $|\Psi_i^{(+)}\rangle$ with a symmetrized state $(1/\sqrt{6})\mathscr{S}|\Psi_i^{(+)}\rangle$, where $\mathscr{S}$ is a sum of 3! permutations. By multiplying the rate by 3, taking into account the three different final states with each of the bound pairs 2-3, 1-3, or 1-2, the following transition probability is found [6]:

$$\omega_{fi}=\frac{\pi}{\hbar}\frac{(2\pi\hbar)^6}{\mathscr{V}^2}\sum_{vlm}\int d\vec{q}_f|\langle\phi_f|V_{12}+V_{13}|\mathscr{S}\Psi_i^{(+)}\rangle|^2 \times\delta(E_f-E_i). \qquad (5)$$

In a gas of N atoms we have $\binom{N}{3}\simeq N^3/6$ three-particle systems, so that the decay rate equation is given by

$$\frac{dN}{dt}=-3\frac{N^3}{6}\langle\omega_{fi}\rangle_{\text{therm}}. \qquad (6)$$

Here $\langle\ \rangle_{\text{therm}}$ stands for thermal averaging over all initial states. Dividing by the volume $\mathscr{V}$ we find the rate of decay of the density:

$$\frac{dn}{dt}=-Ln^3, \qquad (7)$$

with $L=\langle L(\vec{p}_i,\vec{q}_i)\rangle_{\text{therm}}$ and

$$L(\vec{p}_i,\vec{q}_i)=\frac{m}{6\hbar^2}(2\pi\hbar)^7\sum_{vlm}q_f\int d\hat{q}_f|\langle\phi_f|V(r_{12})+V(r_{13})|\mathscr{S}\Psi_i^{(+)}\rangle|^2. \qquad (8)$$

The summation is over all triplet diatom states, q_f is determined by energy conservation, while the integration is over all directions of $\vec{q}_f$.

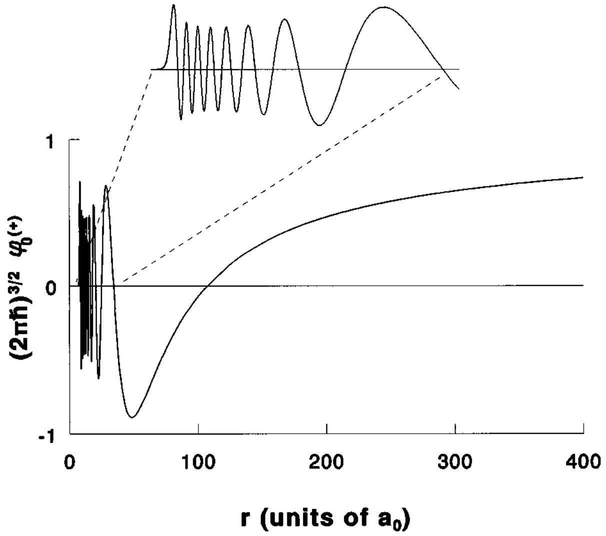

FIG. 2. Two-atom zero-energy scattering state for ^{23}Na. Inset: rapidly oscillating inner part.

B. Zero-temperature limit and Jastrow approximation

We now make use of the fact that the initial state is one with three ultracold atoms, the experimental temperatures in the nK range being small relative to the two-body potentials at the relevant radii $r=O(a)$ in the initial channel as well as to the binding energies of the two-body bound state dominant in the final channels. This allows us to use the $T\rightarrow 0$ limit [15] which implies the replacement $\vec{p}_i=\vec{q}_i=\vec{0}$ in the thermal average: $L=L(\vec{0},\vec{0})$. Thus, to calculate the recombination rate, only the triplet interaction potential, the bound-state wave functions in this potential, and the three-body scattering state $|\mathscr{S}\Psi_i^{(+)}\rangle$ for zero energy are needed. The triplet potential and the bound states for this potential are, at least for Li and Na, easily obtained since accurate potential curves for the ground-state triplet interaction have been constructed [10,11]. The main problem is to find the three-body scattering state, i.e., the solution of the Schrödinger equation $(H_0+V)|\Psi_i^{(+)}\rangle=E|\Psi_i^{(+)}\rangle$ for $E=0$. In the past this state has been calculated rigorously for the case of three hydrogen atoms by means of the Faddeev formalism [6–8]. Even in this case, where the triplet interaction has no bound states, this turned out to be a tedious calculation. In Ref. [7] it was found that the initial scattering state could be well approximated by a Jastrow-like product [16] of three two-atom zero-energy scattering states, $\varphi_0^{(+)}$ (see Fig. 2):

$$\mathscr{S}|\Psi_i^{(+)}\rangle=6\varphi_0^{(+)}(r_{12})\varphi_0^{(+)}(r_{23})\varphi_0^{(+)}(r_{31})(2\pi\hbar)^{3/2}. \qquad (9)$$

Note that the Jastrow form (9) is rigorous when one of the particles is sufficiently far away and that it also fulfills the condition for Bose symmetry. To test the Jastrow approximation we compared the results for calculations of the recombination rate in atomic hydrogen to the results of calculations with the exact initial state for various values of the magnetic field. The difference turned out to be at most 15%. Clearly, because of the existence of many bound diatom states in the triplet potential, the Jastrow approximation will be less accurate in the case of alkali atoms. This will particularly be the case in the part of configuration space where all three particles are close together. In this relatively small part of space, however, the wave function oscillates rapidly and in calculating the final matrix element these oscillations will tend to integrate out.

On the basis of (9) the matrix element in the expression for the rate constant can be written as

$$\begin{aligned}\langle\phi_f|V(r_{13})+V(r_{23})|\mathscr{S}\Psi_i^{(+)}\rangle\\ =\int d\vec{r}\int d\vec{R}\,\varphi_{vlm}^*(\vec{r})\frac{e^{-i\vec{q}_f\cdot\vec{R}/\hbar}}{(2\pi\hbar)^{3/2}}[V(\rho^+)+V(\rho^-)]\\ \times 6\varphi_0^{(+)}(r)\varphi_0^{(+)}(\rho^+)\varphi_0^{(+)}(\rho^-)(2\pi\hbar)^{3/2},\end{aligned}\qquad(10)$$

where $\rho^\pm=|\vec{R}\pm\vec{r}|$. Making use of the properties of the spherical harmonics Y_{lm}, three of the six integration variables, i.e., the Euler angles, defining the orientation of the 1-2-3 triangle in space (see Fig. 1) can be eliminated and we are left with

$$\begin{aligned}\langle\phi_f|V(r_{13})+V(r_{23})|\mathscr{S}\Psi_i^{(+)}\rangle\\ =96\pi^2Y_{lm}^*(\hat{q}_f)\\ \times(i^l)^*\int R^2dR\,j_l(q_fR/\hbar)\int r^2dr\,\varphi_{vl}^*(r)\varphi_0^{(+)}(r)\\ \times\int dx\,P_l(x)V(\rho^+)\varphi_0^{(+)}(\rho^+)\varphi_0^{(+)}(\rho^-)\,\delta_{l,\text{even}}.\end{aligned}\qquad(11)$$

Here $j_l(q_fR)$ is a spherical Bessel function, $P_l(x)$ is a Legendre polynomial, and $x=\cos(\theta)$ with θ the angle between $\vec{r}$ and $\vec{R}$ (see Fig. 1). From this expression it is clear that the free atom in the final state has orbital angular momentum quantum numbers equal to l and $-m$, which is easily understood on the basis of angular momentum conservation: the initial state has total orbital angular momentum $L=0$ and the dimer has quantum numbers l,m. Note that the $V(\rho^+)$ and $V(\rho^-)$ parts of (10) compensate one another for odd l as they should in view of the Bose symmetry under exchange of atoms 2 and 3, while they are equal for even l.

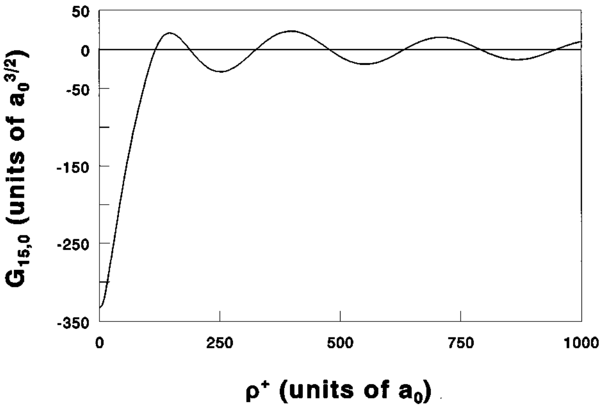

FIG. 3. Integral $G_{vl}(\rho^+)=\int\rho^{-2}d\rho^-\varphi_0^{(+)}(\rho^-)\int dx'j_l(q_fR/\hbar)\times\varphi_{vl}^*(r)\varphi_0^{(+)}(r)P_l(x)$ as a function of ρ^+ for the ^{23}Na$_2$ state $v=15,l=0$.

TABLE I. Partial three-body decay rates for ^{7}Li.

Final state (v,l)	Binding energy (K)	Partial rate L_{vl} (cm^6/s)
10,2	0.337	1.98×10^{-28}
10,0	0.598	2.03×10^{-29}
9,6	1.477	1.29×10^{-30}
9,4	3.279	1.67×10^{-29}
9,2	4.504	1.32×10^{-29}
9,0	5.046	3.75×10^{-32}
8,10	2.711	6.33×10^{-36}
8,8	7.181	4.95×10^{-32}
8,6	10.949	4.05×10^{-31}
8,4	13.829	1.03×10^{-32}
8,2	15.709	6.09×10^{-32}
8,0	16.525	1.07×10^{-30}
7,14	3.077	8.12×10^{-39}
7,12	11.071	2.13×10^{-34}
7,10	18.291	2.57×10^{-30}
7,8	24.504	2.46×10^{-31}
7,6	29.551	1.28×10^{-30}
7,4	33.280	7.16×10^{-31}
7,2	35.763	1.44×10^{-32}
7,0	36.814	1.65×10^{-31}

The expression (11) contains products of rapidly oscillating functions (see Fig. 2), which may easily give rise to numerical problems without a careful choice of integration variables. This indeed turns out to be the case: after carrying out the x integration the integrand of the r integral shows for each fixed value of R rapid and "chaotic" oscillations which are increasingly difficult to handle for increasing atomic mass. The x integral, for instance, involves simultaneous variations of the ρ^+ and ρ^- variables which distort the original regular WKB-like oscillations of the ρ^+ and ρ^- dependent radial wave functions. As a way out, we take the magnitude of the vectors $\vec{\rho}^+$ and $\vec{\rho}^-$ as integration variables, as well as the angle θ' between them:

$$\begin{aligned}\langle\phi_f|V(r_{13})+V(r_{23})|\mathscr{S}\Psi_i^{(+)}\rangle\\ =96\pi^2Y_{lm}^*(\hat{q}_f)(i^l)^*\int\rho^{+2}d\rho^+V(\rho^+)\varphi_0^{(+)}(\rho^+)\\ \times\int\rho^{-2}d\rho^-\varphi_0^{(+)}(\rho^-)\int dx'j_l(q_fR/\hbar)\varphi_{vl}^*(r)\varphi_0^{(+)}\\ \times(r)P_l(x),\end{aligned}\qquad(12)$$

with $x'=\cos(\theta')$. For the dominant bound dimer states close to the continuum the functions $\varphi_{vl}(r)$ and $\varphi_0^{(+)}(r)$ show almost identical fast oscillations, so that in the r interval concerned the resulting local $\sin^2$ function can be replaced by

TABLE II. Partial three-body decay rates for ^{23}Na.

Final state (v,l)	Binding energy (K)	Partial rate L_{vl} (cm^6/s)
15,0	0.002	1.64×10^{-28}
14,4	0.064	1.82×10^{-30}
14,2	0.188	4.56×10^{-30}
14,0	0.246	6.78×10^{-30}
13,8	0.251	1.12×10^{-30}
13,6	0.692	2.16×10^{-30}
13,4	1.035	5.30×10^{-30}
13,2	1.260	2.63×10^{-30}
13,0	1.358	8.61×10^{-31}
12,12	0.389	8.49×10^{-39}
12,10	1.349	1.39×10^{-32}
12,8	2.201	2.31×10^{-33}
12,6	2.905	2.91×10^{-31}
12,4	3.438	9.11×10^{-31}
12,2	3.784	3.74×10^{-31}
12,0	3.933	6.17×10^{-32}

$\frac{1}{2}$. Furthermore, the expression (12) has the advantage that the potential $V(\rho^+)$ which would also disturb the regular oscillations of the integrands of the previous integrations is included in the last integration. Figure 3, which shows the intermediate result of the x' and ρ^- integrations, illustrates the disappearance of the irregular oscillations achieved in this way.

III. RESULTS

In Tables I and II the partial recombination rates are given for the formation of each of the highest two-body bound states of ^{7}Li and ^{23}Na. The partial rates L_{vl} decrease with increased binding energy and also show a systematic decrease at the highest l values considered. Both tendencies can be understood by overlap arguments. Final states which are weakly bound have optimal overlap with the initial state of three slow atoms so that a weaker perturbation operating in a larger part of space is sufficient to induce a transition. For higher orbital angular momenta l the atoms are pushed to larger distances, i.e., the Bessel function j_l is small in a larger radial range, so that the overlap will decrease.

Next we turn to the recombination rate for ^{87}Rb, which is of particular relevance in view of the recent successful BEC experiment. The detailed potential curve for Rb is not yet known, but we know the long range part $(r>30a_0)$ and the locations of the highest bound states relative to the continuum from recent cold-atom photoassociation work [12,13]. This allows us to calculate the three-body rate rather reliably, since the recombination rate tends to be dominated by contributions from larger interatomic distances. This is confirmed by detailed calculations in which we compared recombination rates for a number of different $r<30a_0$ parts of the potential. The latter were obtained from an *ab initio* potential [17], and adjusted to give correct values for the scattering length and highest bound-state energies [13]. We found L to vary by at most a factor of 3. In Table III we present the resulting total recombination rates for ^{7}Li, ^{23}Na, and ^{87}Rb. Note that the decay rate for ^{87}Rb is predicted to be a factor of 50 smaller than that for the two other atoms, which clearly is of great importance for Bose-Einstein condensation experiments.

TABLE III. Total three-body decay rates.

Atom	L (cm^6/s)
^{7}Li	2.6×10^{-28}
^{23}Na	2.0×10^{-28}
^{87}Rb	4×10^{-30}

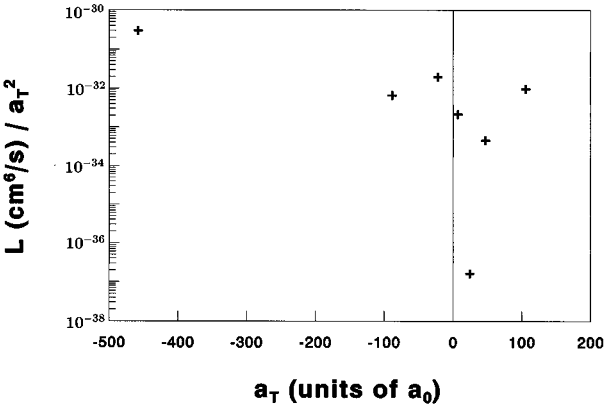

FIG. 4. Value of the partial recombination rate $L_{15,0}$ divided by the square of the scattering length as a function of the value of the triplet scattering length.

The fact that L apparently depends only on the tail of the potential might imply that it could be expressed as a simple function of the scattering length. A simple dependence on a_T is indeed suggested by Eq. (12). If the intermediate result of the x' and ρ^- integrations is considered as constant in the relevant ρ^+ region then the ρ^+ integral $\int\rho^{+2}d\rho^+V(\rho^+)\varphi_0^{(+)}(\rho^+)$ is just the expression for the zero-energy T matrix, which is equal to the two-body scattering length. Detailed calculations show that the amplitude of the intermediate result of the x' and ρ^- integrations depends only weakly on the scattering length for not too extreme values of this latter quantity. A strong dependence of the total L on the scattering length also follows from an even simpler picture of the three-body collision than has been used in the foregoing: the impulse approximation [18]. To facilitate physical insight into this picture we turn to the inverse process of recombination: breakup of a dimer by the collision

TABLE IV. Partial three-body decay rates for ^{23}Na with adjusted potentials.

a_T (units of a_0)	$L_{15,0}$ (cm^6/s)	$L_{15,2}$ (cm^6/s)
106	1.7×10^{-28}	
47	1.0×10^{-29}	
25	9.8×10^{-35}	3.3×10^{-33}
7	1.0×10^{-30}	8.4×10^{-30}
-22	9.5×10^{-30}	4.2×10^{-29}
-88	5.3×10^{-29}	3.2×10^{-27}
-458	6.3×10^{-26}	3.5×10^{-24}

with an atom, for which the transition amplitude is the complex conjugate value. In the picture of the impulse approximation the dimer state is Fourier analyzed as a superposition of all possible relative momentum eigenstates of the two atoms. The ''incident'' atom is affected by each of the states in the superposition separately and collides with one of the atoms only. The transition amplitude to a particular free three-atom state is then equal to the probability amplitude of the dimer relative momentum state multiplied by a two-body scattering amplitude [19]. Since at the relevant low temperatures the latter is equal to the scattering length, the question comes up as to what extent L is proportional to a_T^2. To investigate this for ^{23}Na we varied the scattering length by deepening gradually the inner part of the potential, thereby shifting the radial nodes beyond this range, and calculated the dominant partial recombination rate $L_{15,0}$. The result is shown in Fig. 4. Apparently, there is a considerable scatter around the a_T^2 dependence. In any case Fig. 4 shows convincingly that the recombination rate depends very sensitively on a_T with a tendency to rapidly growing rates for larger $|a_T|$ values. We should stress, however, that it is certainly not the scattering length alone which determines the order of magnitude of the total recombination rate. As the potential is made deeper, at some point it is possible to have a state with $l=2$ as the highest bound state. The partial decay to this state then becomes the dominant process (see Table IV).

IV. CONCLUSIONS

We have calculated the three-body decay rate for doubly-spin-polarized ultracold gas samples of ^{7}Li, ^{23}Na, and ^{87}Rb based on two-body collision information which has recently become available for the above atomic species on the basis of spectroscopic data and cold-atom photoassociation experiments. These atomic species play a key role in the recent BEC experiments. Experimental results [1] indicate that three-body recombination is an important process in these experiments, the loss rate determining the lifetime of the condensate probably being a result of this mechanism. In view of the ultralow temperatures obtained experimentally we approximate the rate L by that in the $T \to 0$ limit. L is a sum over partial rates for formation of the various dimer rovibrational states and is dominated by one or a few of the highest bound states. Note that the recombination rate in a Bose condensate has to be divided by six because of Bose statistics [20].

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