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Conditions for Bose-Einstein condensation in magnetically trapped atomic cesium

E. Tiesinga, A. J. Moerdijk, B. J. Verhaar, and H. T. C. Stoof
Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

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We study conditions necessary for the observation of Bose-Einstein condensation in a magnetically trapped sample of atomic Cs gas. These conditions are associated with the value of the elastic scattering length, the rate of elastic scattering events, and the lifetime for decay of the density due to both magnetic dipole relaxation in two-body collisions, as well as recombination to Cs_2 in three-body collisions. We find that, on the basis of these conditions, the prospects for observing Bose-Einstein condensation are favorable for a gas of ground-state Cs atoms in the highest state of the lowest hyperfine manifold. In all calculated elastic and inelastic two-body rates we find a pronounced resonance structure, which can be understood in terms of the interplay between the singlet-triplet interaction and the hyperfine, Zeeman, and magnetic dipole interactions. The experimental observation of these resonances may help to eliminate present uncertainties about interaction potentials.

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Rapid developments in techniques to cool and manipulate atoms offer new opportunities for many fascinating applications, such as atom interferometry, atomic resonators, atomic fountains, and Bose-Einstein condensation (BEC) in a weakly interacting Bose gas. Although less easy to manipulate than charged particles, atoms have the advantage that the number of particles dealt with simultaneously can be large without significant mutual perturbation. This makes it possible to improve the signal-to-noise ratio in these experiments, and in the case of BEC to make the phase transition more easily attainable by raising the critical temperature. There is, however, a limit to this possibility. We have shown recently [1], that ground-state atom collisions provide a strong limitation to the anticipated improvement of the accuracy and stability of the Cs atomic fountain clock [2]. Also in the case of BEC atomic collisions play a decisive role in determining the conditions for practical realizability. This has become clear during more than a decade of work on spin-polarized atomic hydrogen [3,4]. The same is true for atomic cesium, which has more recently been recognized as a suitable candidate due to its favorable optical cooling properties. The most promising strategy [5] appears to be to precool a Cs gas sample, followed by evaporative cooling in a magnetic trap, which avoids the detrimental role of the radiation trapping force [6] and the photon recoil in (magneto-)optical traps.

An essential ingredient for the BEC phenomenon is a positive value of the scattering length a for elastic two-body collisions of atoms in the selected hyperfine state [7], which makes the atom-atom interaction effectively repulsive. Second, the elastic collision rate should be large enough: Elastic collisions are essential for evaporative cooling by restoring thermal equilibrium after the escape of fast atoms and thus for quenching the system into the critical region of the BEC phase transition, after which the ground state is macroscopically populated [8]. Third, the decay of the density due to inelastic two-body collisions and due to recombination to Cs_2 in three-body collisions should be slow enough. In this paper we will investigate how well the question of the validity of these conditions can be answered on the basis of present knowledge of interaction potentials, excluding the accidental situation of a vanishing triplet scattering length or a triplet bound state at zero energy.

We start from the effective two-body Hamiltonian [1,9,10]

$$H=\frac{\mathbf{p}^2}{2\mu}+\sum_{i=1}^{2}(V_i^{\mathrm{hf}}+V_i^Z)+V^c+V^d, \tag{1}$$

with hyperfine and Zeeman terms

$$V^{\mathrm{hf}}=\frac{a}{\hbar^2}\mathbf{S}^e\cdot\mathbf{S}^N,\quad V^Z=(\gamma_e S_z^e-\gamma_N S_z^N)B \tag{2}$$

for each of the atoms, a central interaction

$$V^c=V_0(r)P_0+V_1(r)P_1, \tag{3}$$

consisting of singlet and triplet terms with P_0 and P_1 projection operators on the singlet and triplet subspaces, and a magnetic dipole-dipole interaction V^d with electron-electron and electron-nucleus parts. Symmetry considerations show that the so-called exchange transitions, induced by the central interaction conserve the orbital angular momentum quantum numbers l and m_l, as well as the total spin projection $M_F=m_{F_1}+m_{F_2}$. The dipole-dipole interaction which is much weaker than the exchange interaction and therefore has little effect on exchange transitions, induces dipole transitions conserving m_l+M_F and satisfying $|\Delta l|=0,2$.

As in our previous paper on the cesium fountain [1], we use a spectroscopically determined singlet potential, taken from Ref. [11]. Presently, there are no comparable data available for the triplet potential. Therefore, we follow the procedure of Ref. [1]. Beyond $r=r_t=15.6a_0$ $V_1(r)$ is determined from the singlet potential by reversing the exchange contribution. For smaller r it is taken from an *ab initio* calculation by Krauss and Stevens [12]. Both singlet and triplet potentials are supplemented with a retardation correction [13] at very large interatomic distances of the order of the wavelengths of optical transitions. The modification consists essentially in a more rapid falloff, proportional to $1/r^7$ instead of the usual van der Waals $1/r^6$ behavior.

We rigorously solved the coupled channel equations in the SM_SIM_I basis, with **S** the total electron spin and **I** the total nuclear spin, up to a radius r_0 of about $80a_0$ beyond which the exchange part of the central interaction is negligible and the radial wave functions of closed hyperfine channels are sufficiently small. Transforming from the SM_SIM_I to the hyperfine basis, we integrated the radial equations of the open hyperfine channels from r_0 to a radius of order $(1000-1500)a_0$, where the central interaction is negligible. For even larger radii the dipole interaction with its long range still contributes significantly to the scattering matrix and was included in first order. The low temperatures prevailing in the magnetic trap allow us to calculate the thermally averaged inelastic scattering rates in the $T=0$ limit. For elastic processes the rates show their limiting $T^{1/2}$ behavior. The Bose character of the Cs atoms thus implies that only symmetric spin states are relevant.

Let us now turn to the first of the above-mentioned conditions for BEC. In view of the selection rules of the exchange interaction a doubly polarized gas of Cs atoms in the highest low-field-seeking hyperfine state can only decay via the weak dipole interaction. In analogy to the case of atomic hydrogen [14], this state may thus be suitable for the observation of BEC. Unfortunately, it turns out that due to the uncertainty in the triplet potential for $r<r_t$, the sign of the scattering length a for elastic scattering of two $(F,m_F)=(4,+4)$ atoms is uncertain. On the basis of present knowledge it is therefore not clear whether BEC is possible in this hyperfine state. However, the Cs hyperfine diagram contains a second long-lived low-field-seeking state with $|m_F|=F$, absent in atomic hydrogen. The importance of this highest state of the lowest hyperfine manifold was recently stressed by Wieman *et al.* [5]. In contrast to the doubly polarized situation, the scattering length of two (3,−3) atoms depends on the applied magnetic field and appears to have a resonance structure. From a number of coupled-channel calculations for different potentials within the range of uncertainty indicated in Ref. [1], we conclude that a is either positive over a long range of fields or positive in narrow field ranges at the positions of the stronger resonances. Taking into account the order of magnitude, 5×10^{-4} T, of the resonance widths, it seems that a field configuration suitable for BEC can be chosen.

Next we estimate the time of decay of the atomic density due to magnetic dipole relaxation. In Fig. 1 we present the field dependence of the $T=0$ rates for the decay of the $(4,+4)$ state. The values for the transitions to the symmetrized two-atom spin states, $\{F_1m_{F_1},F_2m_{F_2}\}=\{44,43\}$, $\{44,42\}$, and $\{43,43\}$, decrease at low B due to the approach to the threshold in the final channel [9]. The transitions to the states $\{44,42\}$ and $\{44,32\}$ are strongly suppressed due to their spin structure which forbids a direct electron-electron dipole transition and take place via higher order, as well as via the much weaker electron-nucleus dipole interaction. Figure 2 shows the dominant rate for the dipole decay of a gas of atoms in the $(3,-3)$ state: that for $\{3,-3,3-3\}\rightarrow\{3,-3,3,-2\}$. As expected, this rate, like the two remaining dipolar rates for this hyperfine state, shows a final channel threshold behavior for $B\rightarrow0$. It should be noted that the suppression due to the $l=2$ centrifugal barrier is less for the $1/r^3$ dipole interaction than it would have been for a typical short-range interaction. For this reason the total $(3,-3)$ decay rate is

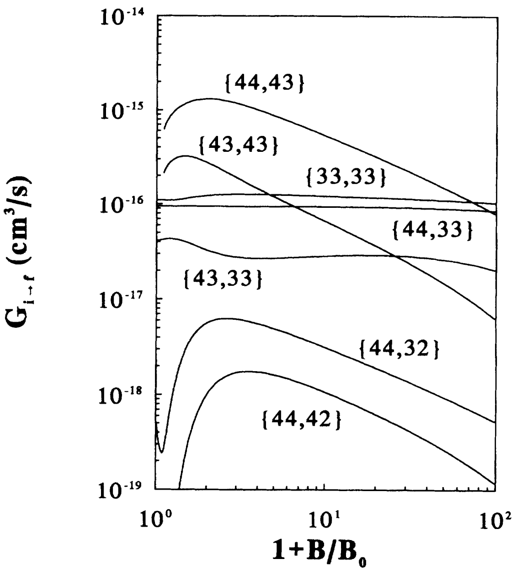

FIG. 1. $T=0$ dipolar relaxation rates $G_{i\rightarrow f}$ for the doubly polarized cesium gas as a function of magnetic field. The horizontal scale shows a gradual transition from a linear to a logarithmic field dependence as we plot $1+B/B_0$ logarithmically. Here $B_0=a/160\mu_B=1.02\times10^{-3}$ T, where the factor $\frac{1}{160}$ ensures a favorable separation between linear and logarithmic parts.

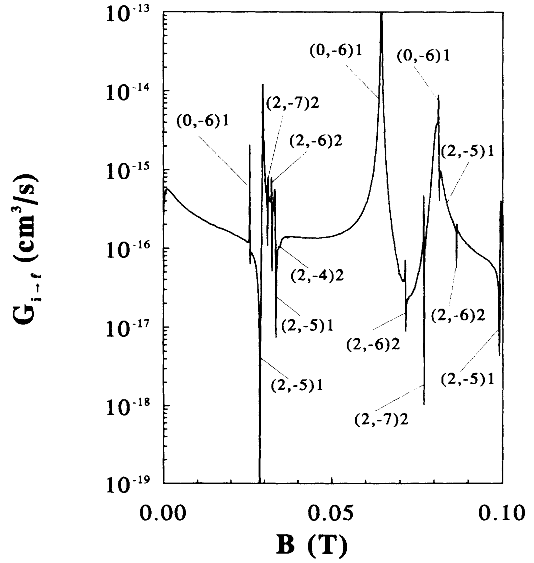

FIG. 2. $T=0$ dipolar relaxation rate G for the transition $\{3-3,3-3\}\rightarrow\{3-3,3-2\}$ as a function of magnetic field. The labels $(l,M_F)i$ denote the quantum numbers of the resonance and the order of the dipolar interaction needed to couple the resonant state to the initial and final channels.

less suppressed relative to that for $(4,+4)$ than one might have expected intuitively. Nevertheless, a definite advantage of the $(3,-3)$ hyperfine state is the greater flexibility associated with the field dependence.

From the order of magnitude of the total decay rate we find a lifetime of order $10^{15}[n\ (\mathrm{cm}^{-3})]^{-1}$ sec, both for $(4,+4)$ and $(3,-3)$. For a typical BEC temperature-density combination, 20 nK and $10^{12}\ \mathrm{cm}^{-3}$, at which experimental attempts are aiming [5], the estimated decay time is of order 10^3 sec. This should be compared with the rate of elastic collisions which our coupled-channel calculations show to be of order $10^{-11}[T\ (\mu\mathrm{K})]^{1/2}$, corresponding to a time of order 1 sec between collisions at the above BEC temperature-density combination.

The most prominent feature of the decay rates for $(3,-3)$ is their resonance structure, which we already mentioned in connection with the sign of a. A more detailed study shows the resonances to be associated with Feshbach quasibound states, belonging to subspaces with definite values of l and M_F. Neglecting V^d, these subspaces are uncoupled. The resonance structure is the continuation to higher energies of the hyperfine-mixed singlet and triplet states spectroscopically observed in the Cs_2 spectrum [15]. Due to the strong hyperfine coupling in Cs combined with the small energy distance between these higher rovibrational singlet and triplet levels, this mixing is a complicated phenomenon which cannot be treated in perturbation theory. The quantum numbers of the resonances have been determined by comparing their strengths in the various channels, as well as by carrying out reduced coupled-channel calculations in separate (l,M_F) subspaces with $V^d=0$. In Fig. 2 we have added the (l,M_F) quantum numbers thus obtained for the various resonances, as well as the total order of V^d needed to couple them to the initial and final channels. Resonances do not occur in the decay rates of the doubly polarized state in Fig. 1. This can be understood in terms of the absence of an (l,M_F) subspace without open channels. We come back to the interpretation of the resonances in a future paper.

Finally we consider the three-body recombination rate in a $(4,+4)$ Cs gas. We calculated the zero-temperature limit of the rate constant [16]:

$$L=\frac{m_{\mathrm{Cs}}}{9\hbar^2}(2\pi\hbar)^7\sum_f q_f\int d\hat{\mathbf{q}}_f|\langle\phi_f|\{V^c(r_{13})+V^c(r_{23})\}|S\psi_i^{(+)}\rangle|^2 \tag{4}$$

where $|\psi_i^{(+)}\rangle$ is the exact zero-energy scattering state for three incoming atoms and S the unnormalized symmetrization operator. The final state $|\phi_f\rangle$ describes a triplet molecule formed by atoms 1 and 2, and the free atom 3 with momentum $\mathbf{q}_f$ relative to the molecular center of mass. The normalization of $|\psi_i^{(+)}\rangle$ and $|\phi_f\rangle$ is described in Ref. [16]. The summation is over all triplet Cs_2 molecular states, q_f is determined by energy conservation, while the integration is over all directions of $\mathbf{q}_f$. The most difficult task in estimating L is the calculation of $|\psi_i^{(+)}\rangle$. We have approximated it by a Jastrow-like product of three two-atom zero-energy triplet scattering states. In the case of the zero-energy scattering state of three doubly polarized hydrogen atoms this turned out to be an excellent approximation to the exact three-body state [17]. Here it is also expected to be a good approximation because the Jastrow-like product is essentially exact in that part of configuration space, which dominates the transition matrix element. We find $L=5\times10^{-29}\ \mathrm{cm}^6/\mathrm{sec}$. The two-atom spin state in a $(3,-3)$ gas being predominantly $S=1$, there is no reason to expect the zero-temperature L value for three $(3,-3)$ atoms to be very different.

A comparison with hydrogen in the doubly polarized $|d\rangle$ state with total dipole decay rate $G\approx10^{-15}\ \mathrm{cm}^3\mathrm{sec}^{-1}$ [9] and recombination rate $L\approx10^{-38}\ \mathrm{cm}^6\mathrm{sec}^{-1}$ [16] clearly shows the enhanced importance of recombination in cesium due to the existence of triplet Cs_2 molecules. For cesium densities above $10^{13}\ \mathrm{cm}^{-3}$ particle loss is dominated by recombination, for lower densities by dipole relaxation. In Fig. 3 we present our estimated two-body and three-body decay times as well as the elastic scattering time as a function of temperature. The density is assumed to have the associated critical BEC value. It appears that in a wide temperature interval a favorable ratio of decay time to elastic scattering time is to be expected. For instance, at the temperature-density combination of 20 nK and $10^{12}\ \mathrm{cm}^{-3}$ the ratio is of order 10^3.

Varying the *ab initio* part of the $S=1$ potential as mentioned previously, it is possible to get an impression of the sensitivity of the calculated rates to the uncertainty in this part of the potential. In this connection note that due to the weakness of the hyperfine couplings relative to the triplet potential for $r<r_t$ the precise shape of $V_1(r)$ is only of importance for the calculated collision quantities

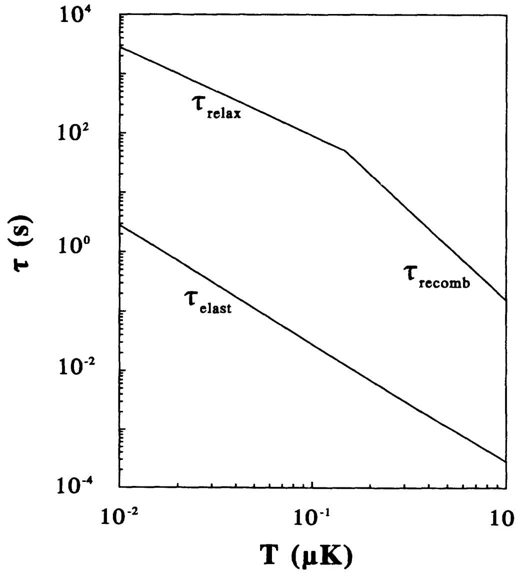

FIG. 3. Elastic and inelastic time scales as a function of the critical temperature.

via one overall parameter per partial wave: the phase of the triplet radial wave function at r_t. The results show that the rates presented above are reliable to within an order of magnitude. The position of the resonances as a function of magnetic field, on the other hand, turns out to be very sensitive, indicating the complicated interplay between the hyperfine and exchange interactions for larger distances where these two interactions are comparable.

In principle, only a few experimental collision quantities are needed to determine the above-mentioned unknown phase parameters for $l=0$ and 2. We expect such data to be available in the near future. If the phases determined from different experimental pieces of information turn out to be contradictory, we will be forced to conclude that ultracold collisions are so sensitive to the fine details of the interatomic potentials that even the careful analysis of Ref. [11] is not adequate for an accurate determination of the singlet and triplet potentials. In this case one may try to avoid an extrapolation of spectroscopic bound-state information to the continuum, by using more direct continuum data in searching for the parameters of the relevant long-range part of the potentials. A comparison of coupled-channel results with elastic scattering and (exchange or dipole) relaxation data will be of great help in this search.

A systematic approach might start with a determination of the absolute value of triplet scattering length a_t by measuring the elastic field-independent rate for $(4,+4)+(4,+4)$ and the $B=0$ elastic rate for $(3,0)+(4,0)$, since both are pure triplet channels. When supplemented with the magnetic-field positions of the pure triplet $M_F=\pm 8$ or ± 7 resonances observed in channels with different M_F, one should be able to determine also the sign of a_t, which, as pointed out above, is a crucial quantity for BEC in a doubly polarized Cs gas sample. Once the relevant long-range parts of the central potentials have been reliably determined, the rates for the dipole transitions may be used to search for an additional spin-spin term with presently unknown magnitude in the $S=1$ ground-state channel due to a second-order spin-orbit effect [18]. Its possible importance was recently pointed out by Julienne, Mies, and Williams [19]. However, preliminary calculations indicate that such a term, which would be concentrated close to the bottom of the triplet potential, is strongly shielded by the final state centrifugal barrier in the case of the $(3,-3)$ state. In the more exothermal decay channels of the $(4,+4)$ state, it might show up and lead to interesting consequences distinguishing ultracold collisions of heavy atoms from those in atomic hydrogen.

In conclusion, we have shown that on the basis of present knowledge of the interaction potentials the conditions for observation of BEC in atomic cesium gas are particularly favorable for the $(3,-3)$ hyperfine state. By a suitable choice of the magnetic-field strength the interatomic interaction can be made effectively repulsive and for a large range of temperatures the thermalizing elastic collisions are much more frequent than inelastic two- and three-body collisions, causing the decay of the gas sample. Furthermore, we predict a pronounced resonance structure in various scattering quantities, which might resolve present uncertainties in the interaction potentials if observed experimentally.

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[1] E. Tiesinga, B. J. Verhaar, H. T. C. Stoof, and D. van Bragt, Phys. Rev. A **45**, R2671 (1992).

[2] A. Clairon, C. Salomon, S. Guellati, and W. D. Phillips, Europhys. Lett. **12**, 683 (1991).

[3] T. J. Greytak and D. Kleppner, in *New Trends in Atomic Physics,* edited by C. Grynberg and R. Stora (North-Holland, Amsterdam, 1984), p. 1125.

[4] I. F. Silvera and J. T. M. Walraven, in *Progress in Low Temperature Physics,* edited by D. F. Brewer (North-Holland, Amsterdam, 1986), Vol. 10, p. 139.

[5] C. Wieman *et al.* (private communication).

[6] T. Walker, D. Sesko, and C. Wieman, Phys. Rev. Lett. **64**, 408 (1990).

[7] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

[8] H. T. C. Stoof, Phys. Rev. Lett. **66**, 3148 (1991); H. T. C. Stoof, Phys. Rev. A **45**, 8398 (1992).

[9] H. T. C. Stoof, J. M. V. A. Koelman, and B. J. Verhaar, Phys. Rev. B **38**, 4688 (1988).

[10] E. Tiesinga, S. J. M. Kuppens, B. J. Verhaar, and H. T. C. Stoof, Phys. Rev. A **43**, 5188 (1991).

[11] H. Weickenmeier, U. Diemer, M. Wahl, M. Raab, W. Demtröder, and W. Müller, J. Chem. Phys. **82**, 5354 (1985).

[12] M. Krauss and W. J. Stevens, J. Chem. Phys. **93**, 4236 (1990).

[13] W. J. Meath and J. O. Hirschfelder, J. Chem. Phys. **44**, 3210 (1966).

[14] A. Lagendijk, I. F. Silvera, and B. J. Verhaar, Phys. Rev. A **33**, 626 (1986).

[15] H. Weickenmeier, U. Diemer, W. Demtröder, and M. Broyer, Chem. Phys. Lett. **124**, 470 (1986).

[16] L. P. H. De Goey, H. T. C. Stoof, J. M. V. A. Koelman, B. J. Verhaar, and J. T. M. Walraven, Phys. Rev. B **38**, 11 500 (1988).

[17] L. P. H. de Goey, H. T. C. Stoof, B. J. Verhaar, and W. Glöckle, Phys. Rev. B **38**, 646 (1988).

[18] S. R. Langhoff, J. Chem. Phys. **61**, 1708 (1974); P. S. Julienne, J. Mol. Spectrosc. **56**, 270 (1975).

[19] P. S. Julienne, F. Mies, and C. Williams (private communication).