

FEW-BODY COLLISIONS IN A WEAKLY INTERACTING BOSE GAS

PROEFSCHRIFT

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Hendricus Theodorus Christiaan Stoof

geboren te Veldhoven

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prof. dr. B.J. Verhaar
en
prof. dr. W. Glöckle**

$$\left\{ \gamma^\mu \partial_\mu - m \right\} \psi(x) = 0$$

"I feel that a theory, if it is correct, will be a beautiful theory, because you want the principle of beauty when you are establishing fundamental laws. Since one is working from a mathematical basis, one is guided very largely by the requirement of mathematical beauty. If the equations of physics are not mathematically beautiful that denotes an imperfection, and it means that the theory is at fault and needs improvement. There are occasions when mathematical beauty should take priority over agreement with experiment. [.....]

A beautiful theory has universality and power to predict, to interpret, to set up examples and to work with them. Once you have the fundamental laws, and you want to apply them, you don't need the principle of beauty any more, because in treating practical problems one has to take into account many details and things become messy anyway."

P.A.M. Dirac

(8 august 1902 - 20 oktober 1984)

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CHAPTER 1:
INTRODUCTION

I. BOSE-EINSTEIN CONDENSATION AS A SPONTANEOUS SYMMETRY BREAKING PHENOMENON

The initial successes of quantum mechanics were associated with systems having a finite number of degrees of freedom. The successful explanation of the properties of such systems led to a general belief in the correctness of the quantum mechanical theory. Very different phenomena have since then been explained without modifications of the basic formalism. However, there are physical phenomena, known collectively as macroscopic quantum effects, whose explanation requires the extension of quantum mechanics to systems with an infinite number of degrees of freedom. The first developments leading to this extension of quantum mechanics, which is sometimes called QM_{∞} , date from the fifties.¹ Recent monographs by Strocchi² and Sewell³ summarize the present status of QM_{∞} .

One of the phenomena typical for infinite quantum systems is spontaneous symmetry breaking. Suppose that the system under consideration possesses a symmetry, because the Hamiltonian is invariant under the transformations of a group \mathcal{G} . In the case of quantum mechanics with a finite number of degrees of freedom this implies that the (in most cases unique) ground state is also invariant. However, for QM_{∞} we have in general a set of inequivalent ground states and all we deduce from the symmetry of the system is the invariance of the complete set and not necessarily of an individual element. As a consequence the symmetry may be broken spontaneously: Although the dynamics of the system is symmetric, its ground state may not have this property. However, the possible ground states are connected to each other by the elements of the symmetry group \mathcal{G} .

An important example in elementary-particle physics is the $U(1) \times SU(2)$ electroweak gauge theory, in which spontaneous symmetry breaking in combination with gauge invariance gives rise to the mass of intermediate vector bosons and of spin $\frac{1}{2}$ particles.⁴ Another example, which we discuss below, is Bose-Einstein condensation,⁵ associated with a macroscopic occupation of the one-particle ground state in a gas of weakly interacting bosons. To place the latter example in the wider context of QM_{∞} it is useful to sketch briefly some aspects of this general theory. For a more systematic introduction we refer to the Refs. 2 and 3.

The differences between QM_{∞} and the quantum theory involving only a finite number of degrees of freedom can be traced back to the following theorem due to Von Neumann.⁶ In the case of a finite system the algebra \mathcal{A} of the coordinates q_{α} and conjugate momenta p_{α} , obeying the commutation relations

$$\left\{ \begin{array}{l} [q_\alpha, q_\beta]_- = 0, \quad [p_\alpha, p_\beta]_- = 0 \\ [q_\alpha, p_\beta]_- = i\hbar\delta_{\alpha\beta} \end{array} \right. \quad (1)$$

has only irreducible representations which are (unitarily) equivalent to the usual Schrödinger representation $p_\alpha = -i\hbar\partial/\partial q_\alpha$ on the Hilbert space of square-integrable functions. Since a unitary transformation does not change the expectation values of physical quantities the choice of a representation is just a matter of convenience. However, in QM_∞ the algebra \mathcal{A} has inequivalent irreducible representations. The various representations can generally be distinguished by means of a macroscopic quantity, commuting with the complete algebra \mathcal{A} and consequently reducing to a constant in an irreducible representation. Due to this the different representations correspond to macroscopically distinct classes of states of the system, which may have very different behavior because also the dynamics (the Hamiltonian) depends on the particular representation chosen. As a result QM_∞ displays interesting properties such as macroscopic degeneracy, spontaneous symmetry breaking and phase transitions, which are closely related to each other and are absent in ordinary quantum mechanics.

To be more specific we consider a non-relativistic many-body problem, using second quantization and formulating the algebra \mathcal{A} in terms of the field operators $\psi(\mathbf{x})$ and $\psi^\dagger(\mathbf{x})$ obeying the usual (anti)commutation relations in the case of (fermions) bosons. For clarity reasons possible indices corresponding to spin degrees of freedom are suppressed. Note that the algebra \mathcal{A} can also be generated by the creation and annihilation operators of definite momentum states, $a^\dagger(\mathbf{k})$ and $a(\mathbf{k})$, respectively. As usual they are related to the field operators $\psi^\dagger(\mathbf{x})$ and $\psi(\mathbf{x})$ by means of a Fourier transform.

For a large class of systems, in particular systems showing superfluid or superconductive behavior, any irreducible representation of \mathcal{A} can be formulated as an operator algebra in a Hilbert space \mathcal{H} , where the latter corresponds to a ground state $|\Psi_0\rangle$ and all its elementary excitations. (Technically this is known as a Fock-representation.) For a characterization of the representation or equivalently the Hilbert space \mathcal{H} with ground state $|\Psi_0\rangle$, we consider so-called Haag-charges of the form

$$\tilde{Q}_{nm}[F] = \lim_{V \rightarrow \infty} \frac{1}{V} \int dx \int dy_1 \dots dy_n \int dz_1 \dots dz_m \times \quad (2)$$

$$\times F(\mathbf{x}; \mathbf{y}_1, \dots, \mathbf{y}_n; \mathbf{z}_1, \dots, \mathbf{z}_m) \psi^\dagger(\mathbf{y}_1) \dots \psi^\dagger(\mathbf{y}_n) \psi(\mathbf{z}_1) \dots \psi(\mathbf{z}_m) .$$

where V is the volume of the system and $F(\mathbf{x}; \mathbf{y}_1, \dots, \mathbf{y}_n; \mathbf{z}_1, \dots, \mathbf{z}_m)$ a localized function,

which vanishes unless y_1, \dots, y_n and z_1, \dots, z_m are in a finite environment of x . Such operators can be shown⁷ to commute with the algebra \mathcal{A} . In an irreducible representation they are equal to a complex constant which can therefore be used to label that representation. In the BCS-theory⁸ of superconductivity a Haag-charge of Q_{02} type plays a central role. It is equal to the well-known "energy gap" in the quasi-particle dispersion relation and can be used to solve this model exactly in the thermodynamical limit.

We now turn to the form of the Haag-charge in the case of Bose-Einstein condensation. Assuming two-body interactions only and denoting the Fourier transform of the interparticle potential by V_q the Hamiltonian of N bosons in a volume V with periodic boundary conditions is given in usual notation by

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} V_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}} a_{\mathbf{k}'} \quad (3)$$

where $\epsilon_{\mathbf{k}}^0 = \hbar^2 k^2 / 2m$ is the kinetic energy of a particle with momentum $\hbar\mathbf{k}$. Following Strocchi,² we take as a Haag-charge

$$Q \equiv Q_{0,1}[\delta] = \lim_{V \rightarrow \infty} \frac{1}{V} \int dx \psi(x) \equiv \lim_{V \rightarrow \infty} \frac{a_0}{\sqrt{V}} \quad (4)$$

and require that the states of the gas form an irreducible representation of \mathcal{A} , so that Q reduces to a constant. Clearly, in the case of a non-vanishing value of Q , we have a macroscopic number of particles with zero momentum and the corresponding representation of \mathcal{A} describes the Bose-condensed phase of the gas. Hence we write Q as

$$Q \equiv \sqrt{n_0} e^{i\vartheta} \quad (5)$$

n_0 being the density N_0/V of condensed particles and in Eq. (4) replace a_0^\dagger by $N_0^{\frac{1}{2}} e^{-i\vartheta}$ and a_0 by the complex conjugate number. This substitution breaks the $U(1)$ gauge symmetry (generated by the particle number operator) of the Hamiltonian. However, as an observable conserving the number of particles, the energy is gauge invariant and independent of ϑ . Thus, in agreement with the general remarks made above, the ground states $|\psi_0(n_0, \vartheta)\rangle$ with different values of ϑ have the same energy and are related to each other by a $U(1)$ gauge transformation.

To find the appropriate Hilbert space of the representation, we neglect terms in the Hamiltonian of the order $N_0^{\frac{1}{2}}$ and N_0^0 , which are small at temperatures near

absolute zero and can be treated by perturbation theory if necessary. The result is

$$H = \frac{1}{2} n_0^2 V_0 + \sum'_{\mathbf{k}} \left\{ \epsilon_{\mathbf{k}}^0 + n_0 V_{\mathbf{k}} \right\} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{n_0}{2} \sum'_{\mathbf{k}} V_{\mathbf{k}} \left\{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger e^{2i\vartheta} + e^{-2i\vartheta} a_{\mathbf{k}} a_{-\mathbf{k}} \right\}, \quad (6)$$

where the prime on the summation symbol means that $\mathbf{k}=0$ is excluded. Diagonalizing this Hamiltonian by means of a (unitary) Bogoliubov transformation⁹ from the particle operators $a_{\mathbf{k}}^\dagger$ and $a_{-\mathbf{k}}$ to the quasi-particle operators $b_{\mathbf{k}}^\dagger$ and $b_{-\mathbf{k}}$ it turns out that the weakly interacting Bose gas behaves as a gas of non-interacting quasi-particles:

$$H \equiv E_0(n_0) + \sum'_{\mathbf{k}} \epsilon_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (7)$$

Here E_0 is the ground state energy and $\epsilon_{\mathbf{k}}$ the quasi-particle energy given by the dispersion relation

$$\epsilon_{\mathbf{k}} = \left\{ (\epsilon_{\mathbf{k}}^0)^2 - n_0^2 V_{\mathbf{k}}^2 \right\}^{1/2}. \quad (8)$$

It is interesting to note that for small values of k the quasi-particles behave like phonons, the dispersion relation being linear in this limit:

$$\epsilon_{\mathbf{k}} \underset{k \rightarrow 0}{\sim} (n_0 V_0 / m)^{1/2} \hbar k \equiv c \hbar k. \quad (9)$$

From a more general point of view these phonon-like excitations are the massless Goldstone modes^{2,4} associated with the broken generator of the $U(1)$ symmetry group.

The many body ground state is defined by $b_{\mathbf{k}} |\psi_0(n_0, \vartheta)\rangle = 0$ for all $\mathbf{k} \neq 0$ and the excited states can be found by application of the quasi-particle creation operators $b_{\mathbf{k}}^\dagger$ to $|\psi_0(n_0, \vartheta)\rangle$. In this way we have been able to construct explicitly the irreducible representation of \mathcal{A} corresponding to the Bose-condensed phase of the system. As mentioned previously this representation is based on a ground state and all its elementary excitations.

II. SPIN-POLARIZED ATOMIC HYDROGEN

The most striking example of the Bose-Einstein condensation process realized experimentally is associated with the superfluid phase of ^4He . Phenomenologically,¹⁰ the characteristics of superfluid helium can be explained by assuming the dispersion

relation of the elementary excitations to be different from a particle-like expression and in particular to be linear for small momenta. To see that this feature indeed leads to superfluidity, we memorize an argument due to Bogoliubov.⁹ Describing the normal part of the quantum fluid below the λ -point as an assembly of non-interacting quasi-particles having an average velocity \mathbf{v} with respect to the condensate and in a state of statistical equilibrium, we find that the average number of quasi-particles with momentum $\hbar\mathbf{k}\neq 0$ and energy $\epsilon_{\mathbf{k}}$ is given by:

$$\langle N_{\mathbf{k}} \rangle = \left[e^{(\epsilon_{\mathbf{k}} - \hbar\mathbf{k} \cdot \mathbf{v}) / k_B T} - 1 \right]^{-1}, \quad (10)$$

where k_B is Boltzmann's constant and T the temperature. The magnitude of \mathbf{v} has an upper limit, because the occupation numbers must be positive. Thus we require for all $\mathbf{k}\neq 0$ that $\epsilon_{\mathbf{k}} > \hbar\mathbf{k} \cdot \mathbf{v}$ or equivalently $\epsilon_{\mathbf{k}} > \hbar k v$.

The upper bound for v is therefore equal to the minimum of the ratio $\epsilon_{\mathbf{k}} / \hbar k$. In the case of the particle-like dispersion relation $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ this implies that v is smaller than $\hbar k / 2m$ for all $\mathbf{k}\neq 0$, i.e. $v=0$. This is what we expect: In thermal equilibrium the fluid as a whole has no velocity or more precisely the normal part of the fluid can have no velocity with respect to the condensate. However, in the case of a linear dispersion relation $\epsilon_{\mathbf{k}} = c\hbar k$ we find only the inequality $v < c$. Hence, the normal part of the fluid can have a stationary (frictionless) flow in an arbitrary direction if the magnitude of the velocity is small enough. Carrying out a Galilei transformation to a coordinate system in which the quasi-particles have zero average velocity both the existence of superfluidity as well as a critical velocity above which the phenomenon cannot take place is explained.

The required linear behavior of the dispersion relation was first derived on the basis of a microscopic theory by Bogoliubov⁷ (along the lines described in the foregoing) and later on by Lee et al.,¹¹ who also considered the $T\neq 0$ properties of the Bose-gas. Since these theories rely on the weakness of the interaction or more precisely on the smallness of the gas parameter $(na^3)^{\frac{1}{2}}$, where n is the density and a the scattering length, they are not able to give a reliable description of the dense ⁴He liquid.

In the last decade a great deal of interest has been devoted to spin-polarized atomic hydrogen gas as a system for which $(na^3)^{\frac{1}{2}}$ is small, because the small atomic mass gives rise to a low critical density above which the condensation takes place. In contrast with helium, the required densities at subkelvin temperatures are so low that essentially only two and three-body collisions are important. Together with the fact that hydrogen is the only element for which the interparticle potentials can be calculated accurately from first principles,¹² it is clear that at least from a

theoretical point of view spin-polarized atomic hydrogen is an ideal candidate for the study of the Bose-Einstein transition and of QM_{∞} effects in general.

Also from an experimental point of view, atomic hydrogen has some desirable properties: It is conveniently manipulated and (electron) spin-polarized using easily obtainable magnetic fields ($B < 10T$) and most importantly it offers the possibility of an independent control of both density and temperature, making the system very flexible. As it turned out the main obstacle towards successful experiments is the strong tendency of the hydrogen atoms to recombine to molecular H_2 on the walls of the container. The actual stabilization of atomic hydrogen was first carried out by Silvera and Walraven¹³ in their pioneering work of 1980. They sufficiently suppressed the recombination by electron-spin polarizing the gas sample and by covering the walls with a superfluid helium film, which has a very weak interaction with hydrogen atoms.

After this breakthrough, opening up a completely new field of research, various other groups throughout the world have contributed substantially to our understanding of the physical properties of the system. We mention explicitly the groups of T.J. Greytak and D. Kleppner at MIT, W.N. Hardy at UBC, S. Jaakkola in Turku, D.M. Lee at Cornell University, I.F. Silvera at Harvard University, J.T.M. Walraven in Amsterdam and more recently the group of I.I. Lukashevich at the Kurchatov Institute in Moscow. For an account of the various contributions and their historical context we refer to the review papers of Greytak and Kleppner¹⁴ and Silvera and Walraven.¹⁵ Here we suffice with a brief summary of the present status in the investigation of atomic hydrogen.

Presently there are two different ways in which one hopes to establish the Bose-condensed state. The first approach is historically the older one and aims at a compression of a gas sample of high-field seekers ($H\downarrow$) in a magnetic field maximum at relatively comfortable temperatures ($T \approx 100-500mK$). However, in this temperature range the required densities are so high that three-body recombination on the surface and in the volume cause a rapid and sometimes even explosive decay^{16,17,18} of the gas. To circumvent this problem Silvera¹⁹ has suggested applying high magnetic fields in combination with negative hydrostatic pressures in conventional experiments based on compression of hydrogen bubbles. Another way out has been put forward by Kagan and Shlyapnikov,²⁰ who propose to use strongly inhomogeneous fields produced by an electric or magnetic needle²¹ to compress only a small part of the total system.

The second approach is based on the idea of trapping hydrogen atoms in free space,²² which makes it possible to achieve much lower temperatures since contact with liquid helium is avoided. In this way the required densities are much smaller and only two-body relaxation processes are of importance. Experimentally, both

static^{23,24} and dynamic^{25,26} magnetic traps seem to be feasible and temperatures in the order of $10\mu\text{K}$ may be in reach using a combination of laser (Lyman- α)²⁷ and evaporative²³ cooling.

Within the framework of the latter trapping approach experimental progress has taken place almost exclusively in connection with the static version. It is of interest for the following to point out that such static traps are based on a spatially inhomogeneous magnetic field operating on the magnetic dipole moments and necessarily confine low-field seekers ($\text{H}\uparrow$). This is due to a theorem, first formulated by Wing,²⁸ according to which it is impossible to create a $|\mathbf{B}|$ maximum in free space. A very direct ad absurdum proof can be based on the equation $\nabla^2 B_z = 0$ with the z-axis pointing in the direction of \mathbf{B} at the position of the field maximum, if that would exist. Clearly, $|\mathbf{B}|$ can only have a maximum if B_z has a maximum. This is, however, impossible due to $\nabla^2 B_z = 0$.

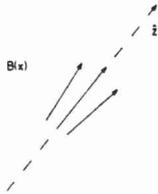


FIG. 1. Magnetic field configuration for a hypothetical absolute maximum of $|\mathbf{B}|$ in free space (see text).

The fact that only low-field seeking atoms can be trapped introduces new decay channels associated with $\text{H}\uparrow \rightarrow \text{H}\downarrow$ transitions induced by two-body collisions. An important part of this thesis is devoted to the theoretical determination of the lifetime of a trapped $\text{H}\uparrow$ gas sample due to such relaxation processes.

Besides this main line of research on spin-polarized atomic hydrogen, a number of phenomena have been and are being studied which are of interest in their own right. Examples are volume²⁹ and surface³⁰ spin waves, the cryogenic hydrogen maser,^{31,32} the interaction of a gas of hydrogen atoms with (almost) resonant electromagnetic radiation^{26,27} and surface physics associated with scattering of hydrogen atoms from a superfluid helium film.^{33,34}

In all above-mentioned cases it is evident that collisions between hydrogen atoms are of utmost importance, because they cause a deviation from the ideal behavior of a Bose-gas. In particular, they are responsible for the decay of the gas and hence for its finite lifetime, placing stringent restrictions on experimental conditions. Therefore, theoretical predictions for the time scales associated with the various collisional processes do not only enhance physical insight but may also point at solutions for experimental problems. The formulation of the appropriate

theory and the numerical evaluation of the decay constants is the main subject of the present thesis.

III. HYDROGEN ATOMS AS COMPOSITE BOSONS

Since a hydrogen atom consists of a proton and an electron, both of which are spin $\frac{1}{2}$ particles, a collision between two or three hydrogen atoms leads in principle to a complicated scattering problem. Additionally, due to the magnetic moments of proton and electron not only the strong Coulomb interaction is important, but also magnetic interactions play a crucial role. In contrast with the Coulomb interaction they are capable of transferring angular momentum among the spin and orbital parts of the system as well as among the electron spin and proton spin parts, giving rise to relaxation and recombination processes that would otherwise be impossible. However, we first solve the Coulomb part of the collision problem and subsequently take the magnetic degrees of freedom into account.

The central question of the present section is the following: How can we derive a description of the collision of hydrogen atoms in terms of "elementary" bosons, taking the required antisymmetry of the wavefunction with respect to permutations of both protons as well as electrons into account exactly? In Sec. IIIA we summarize the solution to this problem in the case of two hydrogen atoms,³⁵ which is based on the adiabatic or Born-Oppenheimer³⁶ approximation. The more complicated case of three hydrogen atoms is treated in Sec. IIIB.

A. Two hydrogen atoms

We adopt the convention to use subscripts for proton and superscripts for electron coordinates throughout and introduce the notation $\mathbf{r} \equiv \mathbf{r}_{12} = \mathbf{x}_1 - \mathbf{x}_2$, $r^{12} = |\mathbf{x}_1 - \mathbf{x}_2|$ and $r_j^i = |\mathbf{x}^i - \mathbf{x}_j|$ for the relative distances. The total Hamiltonian is then

$$H = \sum_i T^i + \sum_i T_i + V^{\text{cou}}. \quad (11)$$

Here, T denotes a kinetic energy and V^{cou} contains all Coulomb interactions between the four charged particles:

$$V^{\text{cou}} = \frac{e^2}{4\pi\epsilon_0} \left\{ \frac{1}{r_{12}} - \sum_{ij} \frac{1}{r_j^i} + \frac{1}{r^{12}} \right\}. \quad (12)$$

The ratio of the proton and electron mass being about 1835, it is an excellent approximation to separate the rapid motion of the electrons from the slow protonic motion and to assume that the state of the electrons follows the position of the protons adiabatically. Mathematically this implies that we first solve the electronic part of the problem for every internuclear distance r separately. Hence, we solve the Schrödinger equation

$$\left\{ \sum_i T_i^e + V^{\text{cou}} - E(r) \right\} |\psi(r)\rangle = 0 . \quad (13)$$

where both the eigenvalue and the eigenstate depend parametrically on r . In addition, we require the total electronic state $|\psi(r)\rangle$ to be antisymmetric under a permutation of electrons and to correspond asymptotically ($r \rightarrow \infty$) to two free hydrogen atoms in a $|1s\rangle$ electronic ground state. The orthogonal solutions are then denoted by $|^{2S+1}\Sigma_{g,u}^{\pm}(r)\rangle |SM_S\rangle$,³⁷ with the subscript "gerade" or "ungerade" depending on the total electron spin having $S=0$ or $S=1$, respectively. (We notice that the electronic wavefunction depends only on the magnitude of r when expressed in body-fixed coordinates.) The corresponding eigenvalues are the well-known^{14,15} singlet and triplet potentials and can for future purposes be written as

$$V^{(S)}(r) = \langle ^{2S+1}\Sigma_{g,u}^{\pm}(r) | \left\{ \sum_i T_i^e + V^{\text{cou}} \right\} | ^{2S+1}\Sigma_{g,u}^{\pm}(r) \rangle . \quad (14)$$

We come back to this point shortly.

The electrons following the motion of the protons adiabatically, a scattering state of the full Hamiltonian (11) with energy E has the form

$$|\psi\rangle = |\phi^{(S)}\rangle |^{2S+1}\Sigma_{g,u}^{\pm}(r)\rangle |SM_S IM_I\rangle . \quad (15)$$

where I , M_I are the quantum numbers for the total proton spin and $|\phi^{(S)}\rangle$ obeys the Schrödinger equation

$$\left\{ \sum_i T_i^p + V^{(S)} - E \right\} |\phi^{(S)}\rangle . \quad (16)$$

determining the protonic part of the wavefunction. Parenthetically we point out that often $V^{(S)}$ is taken to include in addition the expectation value of the nuclear kinetic energy operator in the state $|\psi(r)\rangle$. Because of our interest in the symmetry properties of $|\psi\rangle$, we make the following discussion more transparent by introducing the Heitler-London³⁸ and Shizgal³⁹ approximations. We stress, however, that this

does not affect the symmetry of the states. Within the framework of these approximations we can give the electronic states explicitly:

$$|^{2S+1}\Sigma_{g,u}^+\rangle = \frac{1}{\sqrt{2}} \left\{ |1s\rangle_1^1 |1s\rangle_2^2 + (-1)^S |1s\rangle_1^2 |1s\rangle_2^1 \right\} . \quad (17)$$

using an obvious notation. Substituted in Eq. (14) it leads to the usual³⁷ approximate form of the singlet and triplet potentials in terms of Coulomb and exchange integrals. (Note that in Ref. 37 the Shizgal approximation, which neglects the overlap between the $|1s\rangle_1^1$ and $|1s\rangle_2^1$ states, is not used in order to obtain more accurate potential curves.)

We thus see that $|\psi\rangle$ is indeed antisymmetric under a permutation of the electrons. For $|\psi\rangle$ to be also antisymmetric under a permutation of the protons we require $|\phi^{(S)}\rangle$ to have (even) odd parity if $S+I$ is (even) odd. If we denote the relative orbital angular momentum of the protons by ℓ we can summarize this simply by the symmetry rule: $\ell+S+I = \text{even}$.

Turning to an effective picture in terms of composite bosons we formulate the above-mentioned results as follows. We introduce "mathematical" hydrogen atoms i consisting of electron i and proton i . These atoms have only spin internal degrees of freedom and interact by means of the central interaction V^C defined as

$$V^C = \sum_S V^{(S)} \mathcal{P}^{(S)} , \quad (18)$$

$\mathcal{P}^{(S)}$ being a projection operator on the part of Hilbert space corresponding to atoms with a total electron spin equal to S . The Hamiltonian of the two hydrogen atoms is given by

$$H = H_0 + V^C , \quad (19)$$

where H_0 is the total kinetic energy of the atoms. In analogy to the above treatment $|\psi\rangle = |\phi^{(S)}\rangle |SM_S IM_I\rangle$ is a scattering eigenstate of Eq. (19) with energy E if $|\phi^{(S)}\rangle$ obeys Eq. (16). There is, however, one small difference: the kinetic energy $\sum_1 T_1$ involves the proton mass whereas H_0 involves the hydrogen atom mass. Fortunately, it can be shown³² that non-adiabatic corrections cause a mass renormalization, which gives rise to the replacement of the proton mass by the hydrogen mass.

To make the equivalence between the two pictures complete we now require the wavefunction to be symmetric under permutations of the mathematical hydrogen atoms. As expected this leads to exactly the same symmetry rule as before: $\ell+S+I = \text{even}$.

In this way we have been able to remove the electronic orbital degrees of freedom. They are effectively taken into account in the form of the adiabatic singlet and triplet potentials. Using a generalization of Eq. (14), also magnetic dipolar, Zeeman and hyperfine interactions can now be included in an "effective" form suitable for the composite boson picture. We refer to the thesis of de Goey⁴⁰ for a summary of the final results and now turn to the interesting case of three hydrogen atoms.

B. Three hydrogen atoms

In analogy to the two-body case we apply the very accurate Born-Oppenheimer approximation and solve the extension of Eq. (13) to three electrons and protons:

$$\left\{ \sum_i T^i + V^{\text{cou}} - E(\{\mathbf{x}_i\}) \right\} |\psi(\{\mathbf{x}_i\})\rangle = 0 . \quad (20)$$

which shows the parametric dependence of the solution on the position of the protons. Again the electronic Hamiltonian does not contain the electron spin and the quantum numbers of the total electron spin S are conserved. However, in contrast with the previous section we now have totally symmetric spin states ($S=\frac{3}{2}$) and also spin states of a mixed symmetry ($S=\frac{1}{2}$), instead of totally symmetric and antisymmetric spin states. In the case of mixed symmetry the completely antisymmetric solution of Eq. (20) is not the product of a spin state and a state describing the orbital degrees of freedom but instead a sum of two such products.

Both the $S=\frac{3}{2}$ and $S=\frac{1}{2}$ states are relevant to this thesis, because they correspond to the initial and final states of the dipolar recombination process. Therefore, we will consider both, using again the Heitler-London and Shizgal approximations to make the discussion as transparent as possible and concentrate on the fulfillment of the (anti)symmetry requirements. However, before doing so it is useful to memorize some facts about the permutation group.⁴¹

An irreducible representation of the permutation group can be characterized by the Young-tableau $[\lambda]$, with λ a partition of the number of particles N considered. In the present case of three electrons we have three tableaux $[3]$, $[21]$ and $[111] \equiv [1^3]$, which correspond to a symmetric representation, a two-dimensional representation of mixed symmetry and an antisymmetric representation, respectively. A convenient way to find states that transform according to a D -dimensional (unitary) representation $\Gamma^{[\lambda]}$ of the permutation group is by means of the projection operators:

$$\omega_{\alpha}^{[\lambda]} = \frac{D}{N!} \sum_p \Gamma_{\alpha\alpha}^{[\lambda]*}(p) P . \quad (21)$$

the sum being over all permutations. Crucial for our purpose is the observation that an antisymmetric representation can be formed out of the direct product of $\Gamma^{[\lambda]}$ and the conjugate representation $\Gamma^{[\lambda^{\sim}]}$. Explicitly we have

$$|\psi^{[1^N]}\rangle = \frac{1}{\sqrt{D}} \sum_{\alpha} |\psi_{\alpha}^{[\lambda]}\rangle |\psi_{\alpha^{\sim}}^{[\lambda^{\sim}]}\rangle, \quad (22)$$

where the conjugate partition λ^{\sim} and index α^{\sim} are found by transposition of the Young-tableau $[\lambda]$. For example, if we consider two fermions we have $[2^{\sim}]=[11]$ and Eq. (22) is the obvious statement that the product of a symmetric and an antisymmetric wavefunction is antisymmetric.

After this digression we are now ready to discuss the eigenstates of Eq. (20). First we consider the simple case $S=\frac{3}{2}$. Denoting the total spin of electrons 1 and 2 by s , we have in spin space the symmetric state $|(s\frac{1}{2})SM_S\rangle = |(1\frac{1}{2})\frac{3}{2}M_S\rangle$, belonging to $\Gamma^{[3]}$. In configuration space we therefore need an antisymmetric state

$$\begin{aligned} |\phi^{[111]}(\{\mathbf{x}_i\})\rangle &= \sqrt{6} \omega^{[111]} |1s\rangle_1^1 |1s\rangle_2^2 |1s\rangle_3^3 = \\ &\equiv \sqrt{6} \omega^{[111]} |123\rangle \end{aligned} \quad (23)$$

with spectroscopic designation $1s^3 A_2'$, A_2' standing for the $[111]$ representation and the prime indicating reflection symmetry with respect to the plane of the nuclei. The electronic state then becomes

$$|\psi^{[111]}(\{\mathbf{x}_i\})\rangle = |\phi^{[111]}(\{\mathbf{x}_i\})\rangle |(1\frac{1}{2})\frac{3}{2}M_S\rangle. \quad (24)$$

Calculating the adiabatic energy surface determining the motion of the protons by means of (cf. Eq. (14))

$$V(\{\mathbf{x}_i\}) = \langle \psi^{[111]}(\{\mathbf{x}_i\}) | \left\{ \sum_i T_i^1 + V^{\text{cou}} \right\} | \psi^{[111]}(\{\mathbf{x}_i\}) \rangle. \quad (25)$$

and neglecting the terms giving rise to a three-body force, it turns out that the surface is just the sum of the three triplet pair-potentials, which is equal to

$$V(\{\mathbf{x}_i\}) = \langle (1\frac{1}{2})\frac{3}{2}M_S | \sum_i V_i^c | (1\frac{1}{2})\frac{3}{2}M_S \rangle \quad (26)$$

using the convenient spectator-index notation,⁴² i denoting the pair of atoms (jk) with $j \neq i$ and $k \neq i$. To find the wavefunction of the total system we now have to

supplement (24) with the states $|(1\frac{1}{2})IM_1\rangle$ and $|\phi_s^{(S)}\rangle$, describing the spin and orbital degrees of freedom of the protons, respectively. Furthermore, requiring the complete wavefunction to be antisymmetric under proton permutations we find the (unnormalized) state

$$|\Psi\rangle = (1+P) |\phi_1^{(\frac{3}{2})}\rangle |\psi^{[111]}(\{x_i\})\rangle |(1\frac{1}{2})IM_1\rangle . \quad (27)$$

Here we introduced the operator P , which is the sum of the two cyclic permutation operators of the mathematical atoms.⁴² Together with the symmetry rule $\ell+s+i = \text{even}$ (ℓ is the relative angular momentum of protons 1 and 2) this wavefunction is totally antisymmetric under both electron and proton permutations.

If $S=\frac{1}{2}$ we have two antisymmetric electronic states since we can build two $[21]$ representations, to be distinguished as $[21]'$ and $[21]''$, from the $1s^3$ orbital configuration: This follows from the direct product rule $\Gamma^{[1]} \times \Gamma^{[1]} \times \Gamma^{[1]} = \Gamma^{[3]} + 2\Gamma^{[21]} + \Gamma^{[111]}$. On the other hand for fixed M_S we have only one $[21]$ spin representation. Using the Yamanouchi standard orthogonal representation⁴¹ to obtain the appropriate projection operators we easily find:

$$\begin{cases} |\psi_0^{[111]}\rangle = \frac{1}{\sqrt{2}} \left\{ |\phi_1^{[21]'}\rangle |(0\frac{1}{2})\frac{1}{2}M_S\rangle - |\phi_2^{[21]'}\rangle |(1\frac{1}{2})\frac{1}{2}M_S\rangle \right\} \\ |\psi_1^{[111]}\rangle = \frac{1}{\sqrt{2}} \left\{ |\phi_1^{[21]''}\rangle |(0\frac{1}{2})\frac{1}{2}M_S\rangle - |\phi_2^{[21]''}\rangle |(1\frac{1}{2})\frac{1}{2}M_S\rangle \right\} \end{cases} \quad (28)$$

where we suppressed the parametrical dependence of $|\psi^{[111]}\rangle$ and $|\phi^{[21]}\rangle$ on the position $\{x_i\}$ of the protons. The states $|\phi^{[21]}\rangle$, which are characterized spectroscopically by $1s^3 E'$, can be given explicitly in the Heitler-London approximation:

$$\begin{cases} |\phi_1^{[21]'}\rangle = \frac{1}{\sqrt{12}} \left\{ 2|^{123}\rangle + 2|^{213}\rangle - |^{132}\rangle - |^{321}\rangle - |^{231}\rangle - |^{312}\rangle \right\} \\ |\phi_2^{[21]'}\rangle = \frac{1}{2} \left\{ |^{132}\rangle - |^{321}\rangle - |^{231}\rangle + |^{312}\rangle \right\} \\ |\phi_1^{[21]''}\rangle = \frac{1}{2} \left\{ |^{132}\rangle - |^{321}\rangle + |^{231}\rangle - |^{312}\rangle \right\} \\ |\phi_2^{[21]''}\rangle = \frac{1}{\sqrt{12}} \left\{ 2|^{123}\rangle - 2|^{213}\rangle + |^{132}\rangle + |^{321}\rangle - |^{231}\rangle - |^{312}\rangle \right\} \end{cases} \quad (29)$$

The adiabatic (Born-Oppenheimer) states for $S=\frac{1}{2}$ are found by a diagonalization

of the matrix

$$V_{SS}(\{\mathbf{x}_i\}) = \langle \psi_S^{[111]}(\{\mathbf{x}_i\}) | \left\{ \sum_i T^i + V^{\text{cou}} \right\} | \psi_S^{[111]}(\{\mathbf{x}_i\}) \rangle . \quad (30)$$

In analogy to the discussion of the case $S=3/2$ it can be shown that if we neglect terms leading to a three-body force, Eq. (30) is equal to

$$V_{SS}(\{\mathbf{x}_i\}) = \langle (s\frac{1}{2})\frac{1}{2}M_S | \sum_i V_i^C | (s'\frac{1}{2})\frac{1}{2}M_S \rangle , \quad (31)$$

and the complete six-body wavefunction $|\Psi\rangle$ is a linear combination of the completely antisymmetric states

$$|\Psi_S\rangle = (1+P) |\phi_S^{(\frac{1}{2})}\rangle | \psi_S^{[111]}(\{\mathbf{x}_i\}) \rangle | (i\frac{1}{2})IM_1 \rangle , \quad (32)$$

again with $\ell+s+i = \text{even}$.

Returning to a composite boson picture we notice that due to Eqs. (26) and (31) we are able to remove the electronic orbital degrees of freedom from the description and still obtain the correct Schrödinger equation for $|\phi_S^{(S)}\rangle$ if we use the expected Hamiltonian (cf. Eq. (19)) for three interacting hydrogen atoms

$$H = H_0 + \sum_i V_i^C . \quad (33)$$

and in addition the correspondence

$$\begin{cases} | \psi_S^{[111]}(\{\mathbf{x}_i\}) \rangle \leftrightarrow | (1\frac{1}{2})\frac{3}{2}M_S \rangle \\ | \psi_S^{[111]}(\{\mathbf{x}_i\}) \rangle \leftrightarrow | (s\frac{1}{2})\frac{1}{2}M_S \rangle . \end{cases} \quad (34)$$

If we substitute Eq. (34) in Eqs. (27) and (32), it is clear that in this way we have achieved our objective of reducing the original six-body problem to a three-body problem. The antisymmetry requirement for the electrons and protons constituting the hydrogen atoms is taken into account by using the singlet and triplet pair-potentials and the additional requirement of symmetry of the wavefunction under permutations of the mathematical atoms. Again we are now able to find expressions for an "effective" form of the magnetic interactions with obvious results. Because of the relevance to the dipolar recombination process we note in particular that the electron-electron magnetic dipolar interaction also reduces to the sum of the three interparticle pair-potentials as in Sec. IIIA.

After the above justification of the "elementary particle" treatment of the two and three-atom system it is evident that we can apply formal scattering theory to two and three-body collisional phenomena in a gas of hydrogen atoms. For a mathematically rigorous formulation of this theory we refer to the works of Newton⁴³ and Amrein et al.⁴⁴ A more informal introduction to physically important quantities such as the S(cattering) and T(ransition) matrix, which play a central role in this thesis, is given by Messiah,⁴⁵ Taylor,⁴⁶ Glöckle⁴² and de Goey.⁴⁰ In particular Ref. 40 gives a pedestrian approach to scattering theory using Feynman-like diagrams to clarify the physics involved.

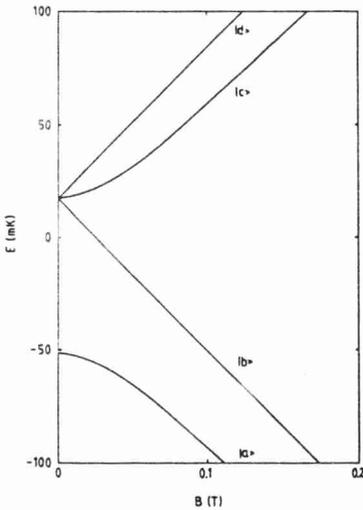


FIG. 2. Rabi diagram of the four hyperfine states of atomic hydrogen in the 1s ground state.

IV. SCOPE OF THIS THESIS

The remaining part of this thesis consists of six publications in the scientific literature. The subjects covered can be grouped into two parts, associated with two and three-body collisional processes, respectively. The first part (Chapters 2 to 4) is in particular relevant to the analysis of relaxational processes in atomic traps, whereas the second part (Chapters 6 and 7) is concerned with three-body recombination, which is the dominant decay mechanism in the high density schemes for the achievement of the Bose-Einstein condensed state.

Chapter 2 is devoted to a study of all possible (exchange and dipolar) relaxation processes, induced by H+H collisions, among the hyperfine states of

atomic hydrogen, which are conventionally^{14,15} denoted by $|a\rangle$, $|b\rangle$, $|c\rangle$, and $|d\rangle$ in order of increasing energy (cf. Fig. 2). The calculation of the rate constants $G_{\alpha\beta\rightarrow\alpha'\beta'}$ of the various relaxation processes is especially important for the analysis of the decay of magnetically trapped atomic hydrogen (H \uparrow). Recently, experiments carried out in Amsterdam by Walraven's group^{24,47} have shown excellent agreement with the results presented in this chapter, when averaged over the magnetic field and density profiles in the trap.

In the case of the cryogenic hydrogen maser it has been shown by our group³² that hyperfine induced effects ultimately limit the frequency stability of the maser and cause a dependence of the frequency shift on the level populations. Therefore, relaxation affecting these populations is also of importance for a detailed study of the hydrogen maser.

In Chapter 3 we explore the possibility of a microwave trap, which was first proposed by Agosta and Silvera⁴⁸ as a way to trap predominantly b-atoms, which are expected to have a much longer lifetime than d-atoms trapped in a static magnetic field minimum. To discuss the finite lifetime of the gas due to collisional processes we are faced with the additional complication of the microwave radiation field. As was pointed out by Julienne⁴⁹ this problem can be solved conveniently if one realizes that the asymptotic states of the scattering process are (two-body) dressed-atom⁵⁰ states. With this in mind we can immediately apply the methods (in particular the degenerate-internal-states approximation⁵¹) of Chapter 2 to find the appropriate decay constants. Chapter 3 is identical to a publication written in collaboration with C.C. Agosta and I.F. Silvera (Harvard University). Although only the calculation of the lifetime in terms of dressed states forms part of this thesis work, we include the full contents of the publication for completeness sake. The principal conclusion is that relatively long lifetimes are obtainable if one is able to use strong microwave fields. However, the main, as yet unsolved, experimental difficulty is connected with the filling of the trap.

The results of Chapters 2 and 3 rely on the fact that the temperature of the gas is much higher than the critical temperature T_c for Bose-Einstein condensation. Hence, the translational degrees of freedom are described by a Maxwell-Boltzmann distribution. In Chapter 4 we drop this restriction and consider the full temperature range and especially $T < T_c$. With the application of magnetically trapped atomic hydrogen (H \uparrow) in mind our primary interest is the calculation of the dipolar relaxation rate constants $G_{dd\rightarrow\alpha\beta}$. We find that at $T=0$ $G_{dd\rightarrow\alpha\beta}$ is a factor of 2 smaller than the nondegenerate result and we even find small differences above T_c for $dd\rightarrow cc$ and $dd\rightarrow dc$ relaxation. These phenomena may be useful for the detection of (the onset of) Bose-condensation. Although the results are based on a homogeneous system, they can easily be extended to the inhomogeneous case. An accurate procedure

is the use of the local-density approximation to calculate the density profile⁵² and subsequently average the rate constants over this profile.

Chapter 5 can be considered as an intermediate chapter, connecting the two and three-body parts of this thesis. It is concerned with the study of the full (also off-the-energy-shell) T(ransition) matrix and gives the momentum space formulation of the effective range theory, which was extended to arbitrary dimensions by our group.⁵³ Although the subject seems somewhat mathematical it is connected to the low temperature behavior of relaxation⁵⁴ and recombination⁵⁵ processes occurring in atomic hydrogen adsorbed on a (superfluid) helium film. In addition, the method proposed may also be useful in the context of nuclear physics since it gives a prescription to find an (in a certain sense) optimal separable approximation to the T-matrix, which is important for the solution of three-body Faddeev⁵⁶ or in general few-body equations.

Finally, Chapters 6 and 7 are devoted to an evaluation of the three-body dipolar recombination rate constant L_g^{eff} for the process $H+H+H \rightarrow H_2+H$ induced by the interatomic magnetic dipolar interaction. This interaction being included as a first-order perturbation, the problem reduces to the calculation of two collision wave functions, one for the initial $H+H+H$ state and one for the final H_2+H state, both including the central interaction exactly. The theoretical formulation used has been described more completely in Ref. 42 and in two previous papers,^{57,58} written by our group in collaboration with W. Glöckle of the University of Bochum. In particular Ref. 58 gives an elaborate discussion of the exact initial state of the recombination process obtained by the solution of the Faddeev equations in momentum space. Moreover, it gives a thorough derivation of the coupled-channels equations which are used in Chapter 6 to analyze the decay of atomic hydrogen at very high magnetic fields.

Historically, the first (approximate) calculation of the dipolar recombination rate was made by Kagan et al.,⁵⁹ in their important paper giving an overview of the various processes leading to decay of spin-polarized atomic hydrogen ($H\uparrow$) at high densities. Although, this calculation gave the correct order of magnitude at about 8T, the magnetic field dependence was in error: Experiments (at that time carried out only below 10T) showed a slight decrease whereas Kagan's model gave a steep increase as a function of magnetic field. Therefore, de Coey et al.⁵⁷ suggested that an additional process (the dipole-exchange mechanism), which was considered to be negligible by Kagan et al., is important at low magnetic field strengths. Because of fundamental problems in the accurate evaluation of this contribution, we decided to start more exact calculations hoping to resolve the existing discrepancies ultimately. To that end we first calculated the exact initial state of three spin-polarized hydrogen atoms with triplet interactions, which confirmed that the

initial state used by Kagan et al. contained the essential physics.

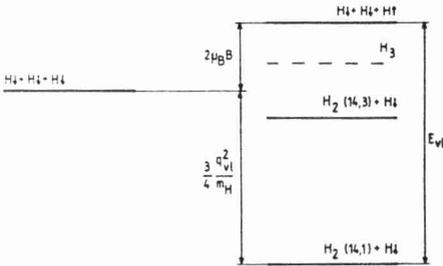


FIG. 3. Energy thresholds for the single spin-flip process, with μ_B the Bohr magneton and q_{vl} the final momentum of the hydrogen atom relative to the H_2 molecule, having rovibrational quantum numbers (v, ℓ) and binding energy E_{vl} . (For the double spin-flip process the loss in Zeeman energy $2\mu_B B$ should be replaced by $4\mu_B B$.)

The following goal was the determination of the final atom-molecule state. However, computational power being limited, an exact approach seemed not to be feasible in this case. Therefore, we decided to follow a two-step approach, which would enhance physical insight in the recombination mechanism. In the first step (Ref. 57 and Chapter 6) we evaluated the contribution of Kagan's dipole mechanism as exactly as possible. In contrast with the approximation of Kagan et al., who neglect all interactions between atom and molecule, we included the possibility of (in)elastic atom-molecule scattering but excluded virtual break-up and most importantly rearrangement, which is directly connected to the dipole-exchange mechanism. Since it turned out that our calculation is not able to explain the experimental data we were led to the conclusion that rearrangement is important and even dominant below 10T.

As a second step we turn in Chapter 7 to a model for the final state, which includes for the first time (in)elastic scattering both with and without rearrangement and neglects only virtual break-up of the molecule. Although there remain serious differences with experiment, our model is able to explain qualitatively both the almost magnetic field independent behavior of L_g^{eff} below 10T and the high values of the recombination rate found in recent experiments⁶⁰ in the field range 10-20T. We believe that these high values are due to states of the long-range H_3 molecule, which give rise to resonances at specific magnetic field strengths, as is shown in Fig. 3. In view of the long-range nature of the molecular states, virtual break-up of the molecule is expected to be very important in obtaining reliable quantitative results. However, including this possibility will only alter the width and the position of the resonance structure but will not change the flat behavior of the background. Therefore, the qualitative picture of the

recombination process given in Chapter 7 is believed to be correct.

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CHAPTER 2:
SPIN-EXCHANGE AND DIPOLE RELAXATION RATES IN ATOMIC HYDROGEN:
RIGOROUS AND SIMPLIFIED CALCULATIONS

Spin-exchange and dipole relaxation rates in atomic hydrogen: Rigorous and simplified calculations

H. T. C. Stoof, J. M. V. A. Koelman, and B. J. Verhaar

Department of Physics, Eindhoven University of Technology, NL-5600 MB Eindhoven, The Netherlands
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We calculate the magnetic field and temperature dependence of the rates for all two-body spin-exchange and dipolar transitions among hyperfine levels in cryogenic H gas by means of the coupled-channels method. A description of this method and its practical application is presented. A simple interpretation of the rates is given, in some cases with associated simple closed-form formulas, based on the degenerate-internal-states approximation.

I. INTRODUCTION

In the past few years spin-polarized atomic hydrogen gas at subkelvin temperatures has attracted a great deal of attention. Already at lower densities the exceptional properties of this gas have shown up via the observation of spin waves.¹ They have also been exploited in successful attempts to construct subkelvin H masers,² with the aim of improving upon the frequency stability of existing atomic frequency standards. The primary interest, however, is still associated with the achievement of the temperature-density regime where effects due to Bose degeneracy are expected to show up. Although Bose- or Fermi-degenerate systems have already been studied extensively in various parts of physics, atomic hydrogen gas promises to be exceptional also from this point of view. In nuclear matter, for instance, the role of occupied levels in damping nucleon collisions within the Fermi sea and thus in explaining the validity of the nuclear shell model is qualitatively clear, but not easily calculated quantitatively owing to the high nucleon density, which makes it difficult to disentangle pure blocking effects from three- and more-particle collisions. A similar remark applies to superfluid helium considered as a Bose-degenerate system.

Degeneracy in polarized atomic hydrogen promises to be realizable in circumstances where average interatomic distances are comparable to the de Broglie wavelength but much larger than the range of interatomic forces, so that the macroscopic occupation of single-particle states will reveal itself in (relaxation and transport) properties describable with pure two-body collisions. The possibility, at least in principle, of independently controllable density and temperature is another attractive feature of Bose-degenerate atomic hydrogen, which distinguishes it from other systems like nuclear matter, superfluid helium, or the electron gas in metals.

Experimental and theoretical work on this topic has had a strong impetus recently by the idea of confining the polarized atomic gas in a magnetic trap, thus avoiding the decay of atomic density by three-body collisions at the helium-covered walls of a gas cell. In a static trap of this kind,³ however, other decay modes arise through

two-body collisions of atoms in the two highest 1s hyperfine states $|c\rangle$ and $|d\rangle$, leading to depolarization via the formation of atoms in the lowest states $|a\rangle$ and $|b\rangle$. A coupled-channels calculation of the associated rates has been presented by Legendijk *et al.*⁴

The purpose of the present paper is threefold. (1) To describe in a more complete form the coupled-channels method, which has been used for the calculation of the H-maser frequency shift⁵ and of the above-mentioned relaxation rates, both due to H+H collisions. (2) To present new values for these rates based on a more accurate numerical calculation and a new H-H singlet potential describing more precisely the experimental data on singlet binding energies. (3) To present a simplified description, in some cases with associated closed-form formulas, for the two-body rates in various regimes of temperature and magnetic field.

Apart from making clear how calculations described in previous papers on the H-maser frequency shifts and on the rates in magnetic traps have been carried out, we believe that the new numerical values as well as the simple closed-form formulas will be extremely helpful for experimental groups working in these areas. For instance, the behavior of the H↑ gas in the first stages of confinement in a trap can be analyzed using the $T \neq 0$ rate constants. Also, for further work on the H maser, the present calculations are of interest. To devise strategies for circumventing the source of frequency instability of the cryogenic H maser, indicated in Ref. 5, it is necessary to know the partial $|a\rangle$, $|b\rangle$, $|c\rangle$, and $|d\rangle$ densities of the hydrogen gas in the cavity. Information about rates for collisional transitions among the hyperfine levels is needed to determine these partial densities theoretically.

In Sec. II A we summarize some equations of scattering theory necessary to derive S - and T -matrix elements for relaxation processes. In Sec. II B we consider the degenerate-internal-states approximation to these elements, and Sec. II C is devoted to the two-body rate equations. In Sec. III we describe our coupled-channels method in a more complete way than has hitherto been done.⁶ The new results for the rates obtained in this way are presented in Sec. IV. We also consider the temperature dependence of some of them and in addition give a

simplified description. Part of this has already been briefly pointed out in a previous paper on atomic deuterium in traps.⁷ Finally, some conclusions are given in Sec. V.

II. TRANSITION AMPLITUDES AND RATES

A. *S* matrix for coupled channels

In this section we summarize some expressions, necessary in the following to calculate the rates and to find simplified expressions for some of them. Although the general structure of the final result for the *S* matrix is obvious from the outset, its normalization has given rise to factor of 2 errors⁶ in connection with $bb \rightarrow ab$ and $ab \rightarrow aa$ relaxation in the case of spin-polarized atomic hydrogen. For that reason it is necessary to define explicitly our conventions with respect to the *S* matrix, as well as the precise normalization of the rate coefficients *G* [cf. the factor $1 + \delta_{\alpha\lambda}$ in Eq. (16)].

We start by considering the collision of two distinguishable particles with internal degrees of freedom, that are described by an internal Hamiltonian H^{int} for each of the atoms with corresponding eigenstates:

$$H^{int}|\alpha\rangle = \epsilon_\alpha |\alpha\rangle. \quad (1)$$

The total Hamiltonian of the two particles in the center-of-mass system is

$$H = \frac{p^2}{2\mu} + \sum_{i=1}^2 H_i^{int} + V \equiv H_0 + V. \quad (2)$$

where *p* is the relative momentum, μ is the reduced mass, and *V* represents the effective interaction among the particles, that may depend on the internal variables and is considered to be of finite range, i.e., *V*(*r*) may be neglected beyond a certain value of *r*. Furthermore, we have introduced the free Hamiltonian H_0 with eigenstates $|\mathbf{p}_{\alpha\beta}\alpha\beta\rangle$ normalized as

$$\langle \mathbf{p}'_{\alpha'\beta'}\alpha'\beta' | \mathbf{p}_{\alpha\beta}\alpha\beta \rangle = \delta(\mathbf{p}'_{\alpha'\beta'} - \mathbf{p}_{\alpha\beta}) \delta_{\alpha'\alpha} \delta_{\beta'\beta}.$$

The associated eigenvalues are

$$E_{\alpha\beta} = \frac{p_{\alpha\beta}^2}{2\mu} + \epsilon_\alpha + \epsilon_\beta. \quad (3)$$

The scattering state $|\Psi_{\alpha\beta}^{(+)}\rangle$, that in a time-dependent picture develops out of the initial state $|\mathbf{p}_{\alpha\beta}\alpha\beta\rangle$, and incorporates all the available information of the scattering process has the familiar asymptotic behavior:

$$\begin{aligned} \langle \mathbf{r} | \Psi_{\alpha\beta}^{(+)} \rangle \sim \frac{1}{(2\pi\hbar)^{3/2}} \left[e^{i\mathbf{p}_{\alpha\beta}\mathbf{r}/\hbar} |\alpha\beta\rangle \right. \\ \left. + \sum_{\alpha'\beta'} \int_{\alpha'\beta'} f_{\alpha'\beta',\alpha\beta}(\mathbf{p}'_{\alpha'\beta'}, \mathbf{p}_{\alpha\beta}) \right. \\ \left. \times \frac{e^{i\mathbf{p}'_{\alpha'\beta'}\mathbf{r}/\hbar}}{r} | \alpha'\beta' \rangle \right], \quad (4) \end{aligned}$$

with $\mathbf{p}'_{\alpha'\beta'} \equiv \mathbf{p}_{\alpha\beta} \hat{\mathbf{r}}$. For the derivation of this equation we

refer to the literature.^{8,9} Furthermore, we have introduced the scattering amplitude for distinguishable particles

$$\begin{aligned} f_{\alpha'\beta',\alpha\beta}(\mathbf{p}'_{\alpha'\beta'}, \mathbf{p}_{\alpha\beta}) &\equiv -\frac{\mu(2\pi\hbar)^3}{2\pi\hbar^2} \langle \mathbf{p}'_{\alpha'\beta'}\alpha'\beta' | V | \Psi_{\alpha\beta}^{(+)} \rangle \\ &\equiv -\frac{\mu(2\pi\hbar)^3}{2\pi\hbar^2} \langle \mathbf{p}'_{\alpha'\beta'}\alpha'\beta' | T | \mathbf{p}_{\alpha\beta}\alpha\beta \rangle, \quad (5) \end{aligned}$$

and also defined the asymptotic magnitude of the momentum in channel $|\alpha'\beta'\rangle$ as

$$p_{\alpha'\beta'} = \sqrt{2\mu(E_{\alpha\beta} - \epsilon_{\alpha'} - \epsilon_{\beta'})}, \quad (6)$$

the square root being positive real (open channels) or positive imaginary (closed channels).

Using the Lippmann-Schwinger equation^{8,9} for $|\Psi_{\alpha\beta}^{(+)}\rangle$ and the notation $G_0(z) = 1/(z - H_0)$ for the free resolvent operator, it is possible to derive the well-known⁸ equation for the *T* operator in Eq. (5):

$$T(z) = V + VG_0(z)T(z), \quad (7)$$

that can, in principle, be solved for arbitrary complex *z*, representing the total energy available to the two-particle system.

Note that in an arbitrary plane-wave matrix element $\langle \mathbf{p}'_{\alpha'\beta'}\alpha'\beta' | T(z) | \mathbf{p}_{\alpha\beta}\alpha\beta \rangle$ no specific relation among \mathbf{p}' , \mathbf{p} , and *z* needs to be fulfilled. This so-called off-shell *T* matrix plays an important role in the three-body problem.⁸ In the present paper where only two-body collisions are considered, it will be more profitable to confine our attention to the on-shell *T* (and *S*) matrix, but to consider it as a function of independent channel momenta $\mathbf{p}'_{\alpha'\beta'}$ of all coupled channels. We return to this in the second part of this section.

The expressions given so far were based on the *p* representation. For actual calculations it is far more convenient to work with angular momenta. We therefore transform to an angular momentum basis $|plm\rangle$ in the momentum space of the particles, defined by

$$\langle \mathbf{p}' | plm \rangle \equiv \frac{\delta(p - p')}{pp'} Y_{lm}(\hat{\mathbf{p}}'). \quad (8)$$

Equation (5) for the scattering amplitude can now be reformulated, introducing the *S* matrix by

$$\begin{aligned} S_{\alpha'\beta'l'm',\alpha\beta lm}(\mathbf{p}_{\alpha\beta}) \\ \equiv \delta_{\alpha\alpha'} \delta_{\beta\beta'} \delta_{ll'} \delta_{mm'} \\ - 2\pi i \mu \sqrt{p_{\alpha\beta} p_{\alpha'\beta'}} \langle \mathbf{p}'_{\alpha'\beta'} l' m' \alpha' \beta' | T | \mathbf{p}_{\alpha\beta} l m \alpha \beta \rangle. \quad (9) \end{aligned}$$

The aforementioned *S* matrix can be proven to be unitary, which corresponds to the conservation of particles. Furthermore, in the case that internal parity is unchanged ($||l - l'|$ is even), it turns out to be symmetrical. To define the *S* matrix symmetrically in all cases, a phase-factor i^l is to be added to every spherical harmonic.¹⁰ We thus find

$$\begin{aligned} \langle r | \Psi_{\alpha\beta}^{(+)} \rangle \sim \frac{1}{(2\pi\hbar)^{3/2}} \left[\sum_{\alpha'\beta'} \sum_{l'm'} \sum_{lm} \frac{2\pi i^l}{i\sqrt{p_{\alpha\beta}/\hbar}} \left\{ S_{\alpha'\beta'l'm',\alpha\beta lm}(p_{\alpha\beta}) \frac{e^{i(p_{\alpha\beta}r/\hbar - l\pi/2)}}{r\sqrt{p_{\alpha'\beta'}/\hbar}} \right. \right. \\ \left. \left. + \delta_{\alpha\alpha'}\delta_{\beta\beta'}\delta_{ll'}\delta_{mm'} \frac{e^{-i(p_{\alpha\beta}r/\hbar - l'\pi/2)}}{r\sqrt{p_{\alpha'\beta'}/\hbar}} \right\} \right] \\ \times Y_{lm}^*(\hat{p}_{\alpha\beta}) Y_{l'm'}(\hat{p}_{\alpha'\beta'}) | \alpha'\beta' \rangle \quad \text{as } r \rightarrow \infty. \quad (10) \end{aligned}$$

We are left with the generalization to identical particles. Because of our interest in atomic hydrogen we will confine ourselves to bosons. It turns out that Eq. (10) is again valid for the symmetrized wave function $\langle r | \mathcal{S} | \Psi_{\alpha\beta}^+ \rangle$, $\mathcal{S} = (1 + \mathcal{P}_{12})$, if we add a factor $2/\sqrt{2 - \delta_{\alpha\beta}}$ to the right-hand side and replace all channel states by symmetrized and normalized states $|plm|\alpha\beta\rangle$ defined by

$$|plm|\alpha\beta\rangle = \frac{|plm\alpha\beta\rangle + (-1)^l |plm\beta\alpha\rangle}{\sqrt{2(1 + \delta_{\alpha\beta})}}. \quad (11)$$

In addition, the right-hand side now contains symmetrized S -matrix elements $S_{|\alpha'\beta'l'm',|\alpha\beta lm}$ and corresponding Kronecker symbols $\delta_{|\alpha'\beta'l',|\alpha\beta lm}$. Equation (10) modified in this way is used in the discussion of the coupled-channels approach in Sec. III.

B. Degenerate-internal-state approximation

In a previous paper we already pointed out briefly the importance of neglecting in a specific way the differences between internal energy levels.⁵ Here we will formulate this approach in a more general form, applicable also for $T \neq 0$. Let us first consider exchange transitions. The general idea is to consider an angular momentum basis T -matrix element as a function of all channel momenta involved. In simplified notation

$$T_{l_f l_i}(p_1, p_2, \dots, p_i, \dots, p_f, \dots, p_n)$$

and to split off factors $p_i^{l_i}$ and $p_f^{l_f}$ pertaining to the low-energy dependence in the initial and final channels, respectively. The remaining factor is approximated by its (in general nonvanishing) value for $p_1 = p_2 = \dots = p_n = p$, for which the limit $p \rightarrow 0$ may be taken, but also a common value $p \neq 0$:

$$\begin{aligned} T_{l_f l_i}(p_1, p_2, \dots, p_i, \dots, p_f, \dots, p_n) \\ = (p_f/p)^{l_f} (p_i/p)^{l_i} T_{l_f l_i}(p, p, \dots, p, \dots, p, \dots, p). \quad (12) \end{aligned}$$

Note that for exchange transitions $l_f = l_i$. Note also that the degenerate-internal-states approximation (usually referred to as adiabatic but also as sudden approximation) is often thought to be a typical high-energy approximation, in the sense that all differences between internal energies should be small compared to the asymptotic kinetic energy. In such a case a choice for p so that it is of the order of the asymptotic channel momenta, is preferable. We already pointed out in Ref. 7, however, that this high-energy condition is too strong.

For dipolar transitions the degenerate-internal-states approximation does not work in the form (12). Due to the long range of the dipole interaction the low-energy behavior of dipolar T -matrix elements does not correspond to the above-mentioned powers of p_f and p_i . It is possible, however, to implement the degenerate-internal-states approximation for dipolar transitions in a different way. In all cases a calculation to first order in V^d is sufficiently accurate, i.e.,

$$T_{|\alpha'\beta'l'm',|\alpha\beta lm} = {}_c \langle \psi_{|\alpha'\beta'l'm'}^- | V^d | \psi_{|\alpha\beta lm}^+ \rangle_c, \quad (13)$$

the subscript c indicating that the corresponding scattering state is distorted by central interactions only. The state $|\psi_{|\alpha'\beta'l'm'}^- \rangle_c$ describes a time-reversed scattering process and therefore obeys incoming asymptotic boundary conditions. We now apply the degenerate-internal-states approximation to initial and final states separately, so that both can be expressed as linear combinations of pure singlet and triplet scattering states. We come back to this in Sec. IV B.

C. Rate equations

In this subsection we present expressions for two-body rate constants in terms of the symmetrized S -matrix elements introduced above. A safe way to derive these, from the point of view of avoiding factor of 2 identical-particle errors, is to make use of a quantum Boltzmann equation that can be derived from the BBGKY hierarchy.³

$$\begin{aligned} \frac{d}{dt} \rho_{\kappa\kappa} + i \left[\frac{\epsilon_{\kappa'} - \epsilon_{\kappa}}{\hbar} \right] \rho_{\kappa\kappa} = n \sum_{\lambda} \sum_{\mu', \nu} \sum_{\mu, \nu} \rho_{\mu'\mu} \rho_{\nu\nu} [(1 + \delta_{\kappa'\lambda})(1 + \delta_{\mu'\nu})(1 + \delta_{\kappa\lambda})(1 + \delta_{\mu\nu})]^{1/2} \\ \times \left\langle \frac{\pi\hbar^2}{2\mu q} \sum_{l', m'} \sum_{l, m} (S_{|\kappa'\lambda|l'm',|\mu'\nu|lm}(q) S_{|\kappa\lambda|l'm',|\mu\nu|lm}(q) \right. \\ \left. - \delta_{|\kappa'\lambda|,|\mu'\nu|} \delta_{l'l'} \delta_{m'm} \delta_{|\kappa\lambda|,|\mu\nu|} \right) \Bigg|_{\text{th}}. \quad (14) \end{aligned}$$

Here ρ represents the one-particle density matrix, normalized according to $\text{Tr}(\rho)=1$, n is the particle density, and q the relative momentum of the colliding pair. The right-hand side contains a thermal average with respect to q . In a previous paper⁵ we used Eq. (14) with the coherence of the a and c states included ($\rho_{ac}=\rho_{ca}^* \neq 0$) as a starting point to derive the spin-exchange frequency shift of the cryogenic H maser. The same equation may serve as a starting point to derive the two-body rate equations. In this case the hyperfine states contribute incoherently:

$$n\rho_{\kappa\kappa} = n_{\kappa}\delta_{\kappa\kappa}. \quad (15)$$

We use the unitarity of the S matrix to express the elastic S -matrix element occurring in Eq. (14) in terms of inelastic ones. This leads to the well-known combination of "in" and "out" terms:

$$\frac{d}{dt}n_{\kappa} = \sum_{\lambda} \sum_{\mu\nu} (1 + \delta_{\kappa\lambda})(G_{\mu\nu \rightarrow \kappa\lambda}n_{\mu}n_{\nu} - G_{\kappa\lambda \rightarrow \mu\nu}n_{\kappa}n_{\lambda}) \quad (16)$$

in which the relaxation constants are given by

$$G_{\alpha\beta \rightarrow \alpha'\beta'} = \left\langle \frac{\pi\hbar^2}{\mu q} \sum_{l',m'} \sum_{l,m} |S_{|\alpha'\beta'\rangle l',m',|\alpha\beta\rangle l,m}(q) - \delta_{|\alpha'\beta'\rangle l',m',|\alpha\beta\rangle l,m}|^2 \right\rangle_{\text{th}}. \quad (17)$$

Equation (17) gives the desired relation between the macroscopic quantities $G_{\alpha\beta \rightarrow \alpha'\beta'}$ and the microscopic S matrix, that can be used to calculate the rate constants of all possible exothermic transitions among the hyperfine states of atomic hydrogen. It is sufficient to consider only these transitions, because the rate constants of a process and its inverse are related by

$$G_{\alpha\beta \rightarrow \alpha'\beta'} = G_{\alpha'\beta' \rightarrow \alpha\beta} e^{-(\epsilon_{\alpha'} + \epsilon_{\beta'} - \epsilon_{\alpha} - \epsilon_{\beta})/kT}. \quad (18)$$

III. COUPLED-CHANNELS APPROACH

We start by describing in more detail the effective Hamiltonian (2). Considered as a four-particle problem (two electrons and two protons), a collision between hydrogen atoms is a complicated process. It is well known,⁶ however, that the problem can be considerably simplified by means of the Born-Oppenheimer and Shizgal approximations, which replace the total Hamiltonian by an effective expression (2) in which H^{int} consists of the hyperfine and Zeeman interactions for each of the atoms:

$$H_i^{\text{int}} = \frac{a}{4}\sigma_i^z \cdot \sigma_i^z + \mu_e \mathbf{B} \cdot \sigma_i^z - \mu_p \mathbf{B} \cdot \sigma_i^z \quad (i=1,2) \quad (19)$$

with a the hyperfine constant, μ_e and μ_p the electron and proton magnetic moments, respectively, and σ_i the Pauli spin matrices. The eigenstates of this internal Hamiltonian are conventionally denoted by $|a\rangle$, $|b\rangle$, $|c\rangle$, and $|d\rangle$ in order of increasing energy. In terms of electron (\uparrow) and proton spins (\ddagger) they have the form

$$\begin{aligned} |a\rangle &= \cos\theta | \uparrow \ddagger \rangle - \sin\theta | \uparrow \ddagger \rangle, \\ |b\rangle &= | \uparrow \ddagger \rangle, \\ |c\rangle &= \cos\theta | \uparrow \ddagger \rangle + \sin\theta | \uparrow \ddagger \rangle, \\ |d\rangle &= | \uparrow \ddagger \rangle, \end{aligned} \quad (20)$$

where θ follows from $\tan(2\theta) = a/[2B(\mu_e + \mu_p)]$.

Furthermore, H contains the effective interaction

$$V = V^c + V^d. \quad (21)$$

We use the notation V^c for the central (singlet and triplet) interactions

$$V^c = V_0(r)\mathcal{P}^{(0)} + V_1(r)\mathcal{P}^{(1)}, \quad (22)$$

$\mathcal{P}^{(0)}$ ($\mathcal{P}^{(1)}$) denoting a projection operator on the subspace of singlet (triplet) states. The operator V^d stands for the sum of the electron-electron and electron-proton magnetic dipole interactions. It is a scalar product of operators of rank 2:

$$\begin{aligned} V^d(r) &= -\frac{\mu_0\mu_e^2}{4\pi r^3} \sum_{\mu=-2}^2 \left[\frac{4\pi}{5} \right]^{1/2} (-1)^\mu Y_{2,-\mu}(\hat{r}) \Sigma_{2\mu}^{ee} \\ &\quad + 2\frac{\mu_0\mu_e\mu_p}{4\pi r^3} \sum_{\mu=-2}^2 \left[\frac{4\pi}{5} \right]^{1/2} (-1)^\mu Y_{2,-\mu}(\hat{r}) \Sigma_{2\mu}^{ep}. \end{aligned} \quad (23)$$

The tensor operator Σ^{ij} can be thought of as arising from the coupling of σ^i and σ^j to a spin operator of rank 2. As usual we leave out the proton-proton dipole term.

After this description of the effective Hamiltonian we turn to the problem of solving the time-independent Schrödinger equation. We introduce a fully symmetrical basis of so-called channel states $\{|rlm|\alpha\beta\rangle\}$, similar to Eqs. (8) and (11), and decompose $|\Psi^{(\pm)}\rangle$ as

$$|\Psi^{(\pm)}\rangle = \sum_{|\alpha\beta\rangle} \sum_{l,m} \int_0^\infty dr r^2 \frac{F_{lm|\alpha\beta}(r)}{r} i^l |rlm|\alpha\beta\rangle. \quad (24)$$

In coordinate space we thus find

$$\langle r|\Psi^{(\pm)}\rangle = \sum_{|\alpha\beta\rangle} \sum_{l,m} \frac{F_{lm|\alpha\beta}(r)}{r} i^l Y_{lm}(\hat{r}) | |\alpha\beta\rangle. \quad (25)$$

Substituting this expression into the Schrödinger equation and projecting onto the state $|rlm|\alpha\beta\rangle$ gives the desired coupled-channels equation:

$$\begin{aligned} &\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + \epsilon_a + \epsilon_b - E \right] F_{lm|\alpha\beta}(r) \\ &= - \sum_{|\alpha'\beta'\rangle} \sum_{l',m'} C_{lm|\alpha\beta, l'm'|\alpha'\beta'}(r) F_{l'm'|\alpha'\beta'}(r), \end{aligned} \quad (26)$$

in which the coupling matrix is defined by

$$C_{lm|\alpha\beta, l'm'|\alpha'\beta'}(r) = \frac{\delta(r-r')}{rr'} = i^{l'-l} \langle l'm'|\alpha'\beta' | (V^c + V^d) | r'l'm'|\alpha\beta\rangle. \quad (27)$$

For spin states $\{\alpha\beta\}$ and $\{\alpha'\beta'\}$ with equal total M_F the V^c contribution, if it does not vanish, dominates by far that due to V^d . It is customary to indicate such processes as exchange transitions. Processes to which only V^d contributes are indicated as dipolar transitions. This is the case, in particular, for $\Delta M_F \neq 0$ which requires a transfer of angular momentum among orbital and spin degrees of freedom. For even l also the $\Delta M_F = 0$ transitions with $M_F \neq 0$ belong to this category.

To discuss the numerical method for solving Eq. (26) we introduce a matrix notation

$$\frac{d^2}{dr^2} E(r) = \frac{2\mu}{\hbar^2} C(r) E(r), \quad (28)$$

where the columns of E represent a complete set of linearly independent solutions. The rows correspond to the mutually coupled channels $|lm\{\alpha\beta\}\rangle$. Because of rotational symmetry around the magnetic field direction all of these have the same total magnetic quantum number $M = m + M_F$.

Equation (28) is numerically integrated using a

modified Numerov method.¹¹ During the integration there is a danger of losing sufficient linear independence of the different solutions relative to the numerical noise level. This is caused by the "locally closed" channels, for which $C_{lm\{\alpha\beta\},lm\{\alpha\beta\}}(r) > 0$, leading to exponential growth of one or more common row elements in all columns of E and therefore to numerically linearly dependent solutions. We solve this problem by transforming to new linear combinations of solutions at one or more values of r , thus restoring sufficient linear independence.¹²

From $E(r)$ we extract the S matrix. To that end we introduce two diagonal matrices containing Hankel-like basis solutions of Eq. (28) with the right-hand side equal to 0:

$$I_{mn}(r) = -\delta_{mn} \sqrt{p_m / \hbar i r} h_m^{(-)}(p_m r / \hbar) \\ \sim -\delta_{mn} i e^{-i(p_m r / \hbar - l_m \pi / 2)} / \sqrt{p_m / \hbar} \quad \text{as } r \rightarrow \infty, \quad (29)$$

$$O_{mn}(r) = I_{mn}^*(r).$$

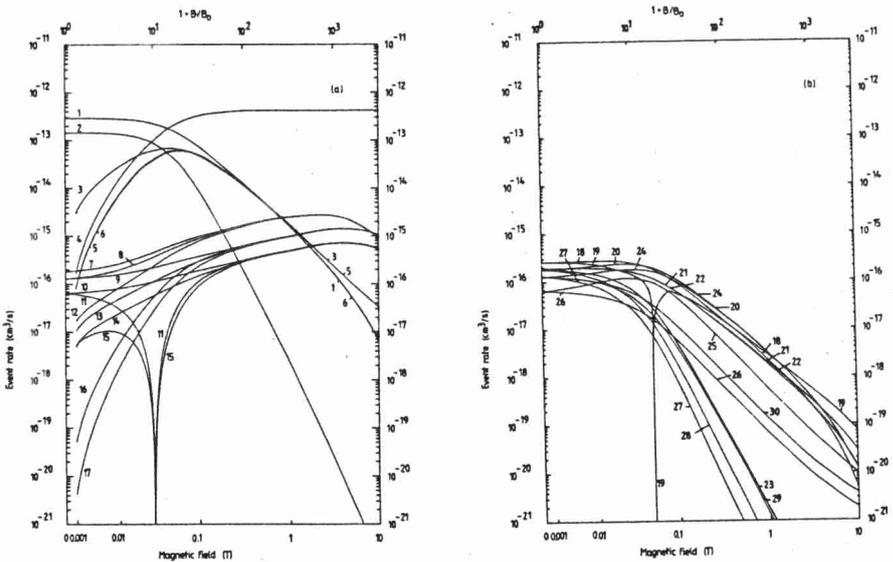


FIG. 1. $T=0$ spin exchange and dipolar relaxation event rates as a function of magnetic field. The horizontal scale shows a gradual transition from a linear to a logarithmic field dependence as we plot $1+B/B_0$ logarithmically. Here $B_0 = a/16\mu_B = 3.17 \times 10^{-3} T$ (μ_B is the Bohr magneton), the factor $1/16$ ensuring a favorable separation in linear and logarithmic parts. The lower horizontal scale shows corresponding values for B . (a) The curves correspond to the following rates: (1): $bd \rightarrow aa$, (2): $cc \rightarrow aa$, (3): $cc \rightarrow bd$, (4): $bd \rightarrow ac$, (5): $cc \rightarrow ac$, (6): $ac \rightarrow aa$, (7): $dd \rightarrow aa$, (8): $cd \rightarrow ab$, (9): $dd \rightarrow ad$, (10): $bd \rightarrow ab$, (11): $cd \rightarrow ac$, (12): $cc \rightarrow bb$, (13): $bc \rightarrow bb$, (14): $cd \rightarrow bd$, (15): $ac \rightarrow ab$, (16): $ad \rightarrow aa$, (17): $cc \rightarrow bc$. (b) The curves correspond to the following rates: (18): $dd \rightarrow ac$, (19): $ac \rightarrow bb$, (20): $cd \rightarrow aa$, (21): $bc \rightarrow ab$, (22): $cd \rightarrow ad$, (23): $bc \rightarrow aa$, (24): $cc \rightarrow ab$, (25): $bc \rightarrow ac$, (26): $bd \rightarrow ad$, (27): $bc \rightarrow ad$, (28): $bb \rightarrow aa$, (29): $cc \rightarrow ad$, (30): $bb \rightarrow ab$. (c) The remaining relaxation rates, not shown in (a) and (b). Curves correspond to the following rates: (31): $dd \rightarrow cd$, (32): $ad \rightarrow ac$, (33): $bd \rightarrow bc$, (34): $ab \rightarrow aa$, (35): $cd \rightarrow cc$, (36): $bd \rightarrow bb$, (37): $ad \rightarrow ab$, (38): $cd \rightarrow bc$, (39): $dd \rightarrow cc$.

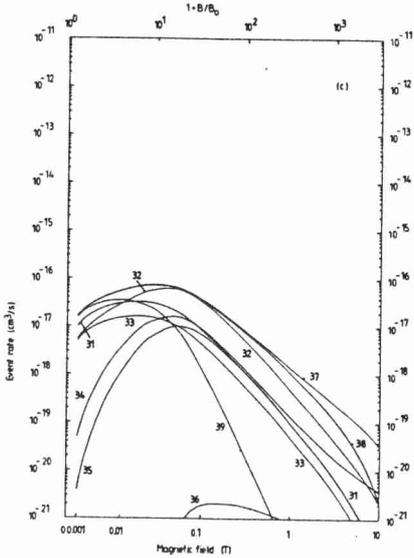


FIG. 1. (Continued).

Here $h_l^{(-)}(\rho)$ is a spherical Hankel function. Again p_m is positive real or positive imaginary. With the help of these matrices the solution $E(r)$ can be written as

$$E(r) = I(r)A(r) + Q(r)B(r). \quad (30)$$

Applying the method of variation of parameters¹³ results in a coupled set of first-order differential equations for the coefficient matrices:

$$\begin{aligned} \frac{d}{dr}A(r) &= \frac{\mu^i}{\hbar^2} Q(r)C(r)[I(r)A(r) + Q(r)B(r)], \\ \frac{d}{dr}B(r) &= -\frac{\mu^i}{\hbar^2} I(r)C(r)[I(r)A(r) + Q(r)B(r)]. \end{aligned} \quad (31)$$

To find the S matrix we integrate the coupled-channels equations (28) until the coefficient matrices in Eq. (30) have become r independent. We then have

$$E(r) = I(r)A + Q(r)B = [I(r) + Q(r)S]A. \quad (32)$$

This defines the S matrix as $S \equiv BA^{-1}$. Comparison with the asymptotic behavior described below Eq. (10) leads to the conclusion that the open-channel submatrix of S so derived, is identical to the S matrix to be calculated.

The application of the above-mentioned procedure would involve an integration to very large radii, because the dipole interaction decreases only as r^{-3} . Therefore, we restrict the integration of Eq. (28) to within a radius of r_1 , beyond which the central interactions can be neglected and treat the dipole interaction in the region $r > r_1$ as a perturbation. We achieve this by defining a local S matrix through the relation $\underline{S}(r) = \underline{B}(r)\underline{A}^{-1}(r)$ and deriving from Eq. (31) an integral equation for $\underline{S}(r)$:

$$\begin{aligned} \underline{S}(r) &= \underline{S}(r_1) - \frac{\mu^i}{\hbar^2} \int_{r_1}^r dr' [I(r') + \underline{S}(r')Q(r')] \underline{C}(r') \\ &\quad \times [I(r') + Q(r')\underline{S}(r')]. \end{aligned} \quad (33)$$

The coupling matrix \underline{C} now contains only the dipole interaction. The first-order treatment then consists of replacing $\underline{S}(r')$ in the integrand by $\underline{S}(r_1)$ and taking the limit $r \rightarrow \infty$.

Because of the strong central interaction it is preferable from a practical point of view to perform the coupled-channels integration in the region $r < r_1$ using the basis $\{|rlmSM_S JM_I\rangle\}$, where the electron spins are coupled to S and the proton spins to I . This basis has as an additional advantage that it is now possible to refrain from the Shizgal approximation by including the electronic spatial degrees of freedom through the use of Heitler-London wave functions. Furthermore, we are now able to include both the intra-atomic as well as the interatomic hyperfine interaction. At $r = r_1$ we finally transform back to the asymptotic (hyperfine) basis and apply Eq. (33) only to the open channels.

IV. RESULTS AND DISCUSSION

A. Coupled channels

In view of magnetic traps for hydrogen atoms with relevant temperatures eventually in the 10–100 μ K range, we present in Fig. 1 the $T=0$ rates

$$G_{\alpha\beta-\alpha'\beta} = 4\pi^3 \hbar^2 \mu p_{\alpha'\beta} |T_{|\alpha'\beta\rangle|l'm\rangle;|\alpha\beta\rangle}|p_{\alpha'\beta}, 0\rangle|^2, \quad (34)$$

for all 45 exothermic spin transitions in H+H collisions as a function of magnetic field. As implied by the theory of Sec. III, the effect of the condensate is left out of consideration. The difference with previous results⁴ is due to a smaller integration step size and an improved H-H singlet potential, describing more accurately the experimental H_2 rovibrational energy data. Although these corrections are rather small, they accumulate in the case of exchange transitions and in some cases lead to significant changes in the rate constants of up to 50%. The changes of the dipolar rates relative to Ref. 4 are only at the 10^{-3} level.

In view of a recent neutral trap experiment³ it is of interest to calculate also the $T \neq 0$ rates for the decay of dd .

In Fig. 2 we present the three most important ones for $B=0$ [(2): $dd \rightarrow ac$; (3): $dd \rightarrow aa$; (4): $dd \rightarrow ad$] and their weighted sum, the loss rate (curve 1). In the following subsection we present simple closed expressions for the B and T dependence of these and other dipolar rates.

As a second application we now consider the cryogenic H maser. In a previous paper⁷ we presented ratelike constants \tilde{G} which govern the maser spin-exchange frequency shift, calculated both by coupled channels and by simplified treatments. Rate constants G of the type considered in the present paper are also of interest for the operation of the H maser. For instance, $bd \rightarrow aa$, $cc \rightarrow bd$, and $cc \rightarrow aa$ processes are of fundamental importance in the description of the cryogenic H maser operating at about 0.5 K. With the usual spin-exchange tuning of the cavity only the part of the H+H collisional frequency shift proportional to the difference $n_a - n_c$ of $|a\rangle$ and $|c\rangle$ atom densities can be eliminated. In order to devise strategies for eliminating fluctuations in the hyperfine-induced collisional part,⁵ which depends in different way on n_a , n_b , n_c , and n_d , it is necessary to calculate the latter from the rate constants $G_{\alpha\beta \rightarrow \alpha'\beta'}$. In calculating these, we neglect the very weak magnetic field within the maser. The results are presented in Fig. 3. We conclude that $G_{cc \rightarrow aa}$ and $G_{bd \rightarrow aa}$ start from nonvan-

ishing values at $T=0$. However, for the transition $cc \rightarrow bd$, which is impossible at zero temperature and magnetic field, the rate increases as $T^{1/2}$ and becomes comparable to $G_{bd \rightarrow aa}$ at the operating temperature of the cryogenic H maser.

B. Simple approaches

For a description of rates in terms of simple approaches it is useful to distinguish three field regimes.

At low magnetic fields ($B \lesssim 0.1$ T) we make use of the fact that differences in internal energies are sufficiently small to apply the degenerate-internal-states approximation. Both the $T \neq 0$ rates of Figs. 2 and 3, and the $T=0$ rates in Fig. 1 (spin-exchange and dipolar) can then be reproduced by simple expressions based on this approximation. Equations (12) and (13) show how the relevant T -matrix elements can then be expressed in terms of pure singlet and triplet quantities: we expand the initial and final spin states in singlet and triplet parts and calculate the separate transition amplitudes using more easily calculable triplet and/or singlet phase shifts and radial wave functions.

For exchange transitions we thus get the simple formulas

$$S_{|\alpha'\beta'\rangle l' m'; |\alpha\beta\rangle l m} = \delta_{l'l} \delta_{m'm} \left(\frac{p_{\alpha'\beta'}}{p} \right)^{l'+1/2} \left(\frac{p_{\alpha\beta}}{p} \right)^{l+1/2} \times \frac{1}{2} \langle \{\alpha'\beta'\} | \mathcal{P}^{(1)} - \mathcal{P}^{(0)} | \{\alpha\beta\} \rangle \{ \exp[2i\delta_l^{(1)}(p)] - \exp[2i\delta_l^{(0)}(p)] \}, \quad (35)$$

$$G_{\alpha\beta \rightarrow \alpha'\beta'}^{cs} = \left(\frac{\pi \hbar^2}{\mu p_{\alpha\beta}} \sum_l (2l+1) \left(\frac{p_{\alpha'\beta'} p_{\alpha\beta}}{p^2} \right)^{2l+1} \sin^2[\delta_l^{(1)}(p) - \delta_l^{(0)}(p)] \right)_{th} |\langle \{\alpha'\beta'\} | (\mathcal{P}^{(1)} - \mathcal{P}^{(0)}) | \{\alpha\beta\} \rangle|^2, \quad (36)$$

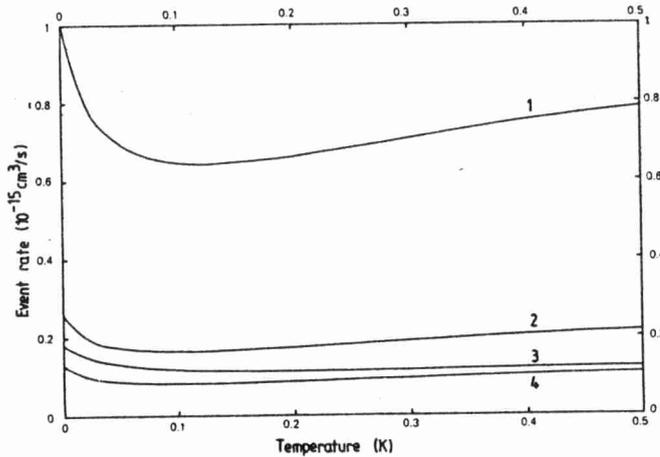


FIG. 2. Temperature dependence of three largest event rates for dipolar decay of dd at $B=0$ [curve 2: $dd \rightarrow ac$, 3: $dd \rightarrow aa$, 4: $dd \rightarrow ad$]. Curve 1: weighted sum (loss rate). Values for $B \neq 0$ follow from Eqs. (42) and (43).

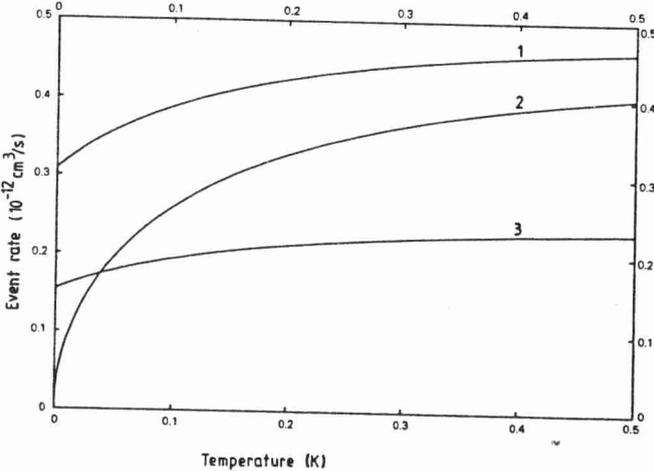


FIG. 3. Temperature dependence of three exchange event rates, important for operation of cryogenic H maser [curve 1: $bd \rightarrow aa$, 2: $bd \rightarrow cc$, 3: $cc \rightarrow aa$]. Coupled-channels curves coincide with result based on closed formula (36).

in which some suitable expression for p in terms of $p_{\alpha\beta}$ and/or $p_{\alpha'\beta}$ can be chosen. In the limit $p \rightarrow 0$ the phase-shifts approach their effective-range limiting values:

$$\sin \delta_i^{(S)}(p) \approx \delta_i^{(S)}(p) \rightarrow -\delta_{10} p a^{(S)} / \hbar, \quad (37)$$

with the scattering lengths denoted by $a^{(S)}$. If this choice is made for $p = p_{\alpha\beta}$ at low T the result is

$$G_{\alpha\beta \rightarrow \alpha'\beta}^{ex}(T=0) = \pi \frac{p_{\alpha\beta}}{\mu} (a^{(1)} - a^{(0)})^2 \times | \langle \alpha'\beta' | | \mathcal{P}^{(1)} - \mathcal{P}^{(0)} | | \alpha\beta \rangle |^2, \quad (38)$$

a result already given in Ref. 7. With the values⁷

$$a^{(1)} = 1.34 a_0, \quad a^{(0)} = 0.32 a_0 \quad (39)$$

for atomic hydrogen inserted, we find agreement with the rigorous $T=0$ rates in Fig. 1 up to $B=0.1$ T to within 10%. The $T \neq 0$ rates in Fig. 3 agree with the simple equation (36) with $p = p_{\alpha\beta}$ to within 5%.

We stress again that the approximation proposed here allows other p values to be chosen. In particular $p^2 = p_{\alpha\beta}^2 + 2\mu(\epsilon_{\alpha} + \epsilon_{\beta} - \epsilon_{\alpha'} - \epsilon_{\beta'})/2$ turns out to lead to highly accurate results. For $B \leq 0.1$ T the results are indistinguishable from the exact ones. Furthermore, even for magnetic field strengths as high as 1 T, the deviations are below the 10% level. We also note that the magnetic field dependence for all exchange rates is governed by factors like $p_{\alpha'\beta'}^{2l+1}$ and by a simple spin matrix element.

Turning to the dipolar transitions we start from Eq. (13) and substitute $V^d = \sum_{\mu} (-1)^{\mu} V_{2\mu}^d \Sigma_{2,-\mu}$ [cf. Eq. (23)]. We find

$$T_{|\alpha'\beta'\rangle l' m', |\alpha\beta\rangle l m} = (-1)^{m'-m} \sum_{S,S'} \langle \psi_{S'l'm'}^{(-)}(p_{\alpha'\beta'}) | V_{2,m'-m}^d | \psi_{S'l'm}^{(+)}(p_{\alpha\beta}) \rangle \langle \alpha'\beta' | | \mathcal{P}^{(S')} \Sigma_{2,m'-m} \mathcal{P}^{(S)} | | \alpha\beta \rangle, \quad (40)$$

allowing evaluation in terms of (mixed) singlet/triplet $1/r^3$ radial integrals. Apparently, the dependence on magnetic field is again located in $p_{\alpha'\beta'}$ and a simple spin matrix element. For the sake of brevity we give here only the spin matrix elements for the subset of dipolar transitions considered in Fig. 2:

$$\begin{aligned} \langle |ac\rangle | \mathcal{P}^{(1)} \Sigma^{ex} \mathcal{P}^{(1)} | | dd \rangle &= 2\sqrt{3} \sin(2\theta), \\ \langle |aa\rangle | \mathcal{P}^{(1)} \Sigma^{ex} \mathcal{P}^{(1)} | | dd \rangle &= 2\sqrt{6} \cos^2 \theta, \\ \langle |ad\rangle | \mathcal{P}^{(1)} \Sigma^{ex} \mathcal{P}^{(1)} | | dd \rangle &= 2\sqrt{3} \cos \theta. \end{aligned} \quad (41)$$

Comparing with the rigorous results in Fig. 1, we find numerically that the deviations are below the 4% level for $B < 0.1$ T and, as expected, increase with increasing field strength. As an illustration of Eq. (40) consider the transition $ac \rightarrow ab$ [curve 15 in Fig. 1(a)]. In this case we obtain

$$\langle |ab\rangle | \Sigma_{2,-1}^{ex} | | |ac\rangle \rangle = \cos(3\theta) / \sqrt{2}$$

and thus $G_{ac \rightarrow ab} \sim \cos^2(3\theta)$. We therefore expect $G_{ac \rightarrow ab}$

to have a sharp minimum at $\theta = \pi/6$, i.e., $B \approx 0.0292$ T. The agreement with our rigorous calculations is excellent.

Without exception the dipolar transitions are far dominated by the single term in Eq. (40) with $S' = S = 1$. This introduces a further simplification: all transition ampli-

tudes contain a common orbital factor which is a "universal" function of $p_{\alpha\beta}$ and $p_{\alpha\beta}$, determined by triplet scattering. A similar conclusion therefore applies to the rates. Writing the energy $\epsilon_a + \epsilon_\beta - \epsilon_{a'} - \epsilon_{\beta'}$ released in a dipolar transition as Δ , we find that for low temperatures ($3k_B T \lesssim \Delta$) the corresponding rate is described by

$$G_{\alpha\beta \rightarrow \alpha'\beta'}^{\text{dip}}(B, T) = (0.2130 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}) (\Delta/a)^{1/2} \times \left[1 - 1.440 \frac{k_B T}{\Delta} + 1.797 \left(\frac{k_B T}{\Delta} \right)^2 \right] | \langle \{ \alpha' \beta' \} | \mathcal{P}^{(1)} \Sigma_{2, m-m'} \mathcal{P}^{(1)} | \{ \alpha \beta \} \rangle |^2 \quad (42)$$

to within 2%. For higher temperatures ($0.2 \lesssim \Delta/k_B T \lesssim 3$) we have

$$G_{\alpha\beta \rightarrow \alpha'\beta'}^{\text{dip}}(B, T) = (0.5741 \times 10^{-17} \text{ cm}^2 \text{ s}^{-1}) (k_B T/a)^{1/2} \times \left[1 + 1.401 \frac{\Delta}{k_B T} - 0.06181 \left(\frac{\Delta}{k_B T} \right)^2 \right] | \langle \{ \alpha' \beta' \} | \mathcal{P}^{(1)} \Sigma_{2, m-m'} \mathcal{P}^{(1)} | \{ \alpha \beta \} \rangle |^2, \quad (43)$$

also to within 2%. It should be pointed out that Eqs. (42) and (43) are also valid for dipolar transitions at stronger fields, provided the energy released in such a transition is not too high. In particular, the high-field behavior of the $bb \rightarrow ab$ and $ab \rightarrow aa$ dipolar transition rates, important quantities in b -state atom experiments, is described by Eqs. (42) and (43) with the spin matrix element equal to $-2\sqrt{3}\mu_p/\mu_e(1 + 16.68/B)$. Equation (43) is a generalization of a closed formula presented previously¹⁴ to a greater set of transitions.

In the intermediate field regime, $0.1 \text{ T} \lesssim B \lesssim 1 \text{ T}$, it is no longer possible to neglect the energy differences between the various hyperfine states because corrections to the T -matrix element to first⁵ and higher order in the internal level splittings become important. It appears that at these intermediate fields the solution of the full coupled-channels equation is required to obtain reliable values of the relaxation constants.

In the strong-field regime ($B \gtrsim 1 \text{ T}$) a simple approach is again possible. This is already evident by a simple inspection of Fig. 1(a). Let us first pay attention to the exchange transitions. These clearly fall in three different categories: they arise essentially from cross terms of exchange and the n th power of the hyperfine interaction, where $n = 0, 1$, or 2 . This expresses itself in three different slopes $\sim B^{-2n}$. To understand this in more detail, we consider the coupling among the channels cc , aa , $\{ac\}$, and $\{bd\}$. Ordering rows and columns correspondingly, the coupling matrix is to lowest nonvanishing order in $\theta \approx a/[B(\mu_e + \mu_p)] \equiv \epsilon$:

$$\begin{pmatrix} V_1 & \epsilon^2(V_1 - V_0) & \frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) & -\frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) \\ \epsilon^2(V_1 - V_0) & V_1 & -\frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) & \frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) \\ \frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) & -\frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) & \frac{1}{2}(V_1 + V_0) & \frac{1}{2}(V_1 - V_0) \\ -\frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) & \frac{1}{2}\sqrt{2}\epsilon(V_1 - V_0) & \frac{1}{2}(V_1 - V_0) & \frac{1}{2}(V_1 + V_0) \end{pmatrix}. \quad (44)$$

Clearly, for strong fields the exchange coupling is in almost all cases damped by (a power of) the hyperfine mixing parameter ϵ and can thus be treated in first order. The only exception concerns $\{bd\}$ and $\{ac\}$, which are strongly coupled mutually in a B independent way. This agrees with Fig. 1(a). The 2×2 submatrix pertaining to these channels decouples if one transforms to $[\{bd\} + \{ac\}]/\sqrt{2}$ and $[\{bd\} - \{ac\}]/\sqrt{2}$ basis states. The diagonal potentials for these states are pure triplet and singlet potentials, respectively. In a sense the degenerate-internal-states approximation is again applicable here for strong fields since the difference between bd and ac internal energies is small. Equations (35) and (36) therefore apply. For $T \rightarrow 0$ we then have in particular

$$G_{bd \rightarrow ac}^{\text{ex}} = \pi \frac{P_{ac}}{\mu} (a^{(1)} - a^{(0)})^2 \cos^2(2\theta). \quad (45)$$

Equation (45) describes the $bd \rightarrow ac$ curve in Fig. 1(a) for all B values to within 4%.

Disregarding $O(\epsilon^3)$ terms it follows also from the matrix (44) that aa and cc are coupled only to the difference channel $[\{bd\} - \{ac\}]/\sqrt{2}$. This explains the coincidence at higher B of the 1 and 6 and of the 3 and 5 curves. In analogy to Eq. (40) we have for these transitions

$$\begin{aligned} T_{|bd\rangle l'm', |cc\rangle lm} &= -T_{|ac\rangle l'm', |cc\rangle lm} \\ &= \delta_{l'l} \delta_{m'm} \frac{1}{2} \sqrt{2} \epsilon \langle \psi_{0lm}^{(-)} | (V_1 - V_0) | \psi_{1lm}^{(+)} \rangle, \\ T_{|aa\rangle l'm', |bd\rangle lm} &= -T_{|aa\rangle l'm', |ac\rangle lm} \\ &= -\delta_{l'l} \delta_{m'm} \frac{1}{2} \sqrt{2} \epsilon \langle \psi_{1lm}^{(-)} | (V_1 - V_0) | \psi_{0lm}^{(+)} \rangle. \end{aligned} \quad (46)$$

Here we used the $SM_S IM_I$ structure of the $\alpha\beta$ states for

strong B .

For weaker fields (but still so strong that the above first-order treatment applies), the singlet and triplet wave functions ψ can both be inserted for zero energy, leading to four T -matrix elements equal in absolute magnitude. This is in agreement with Fig. 1(a): The curves 3,5 and 1,6 coincide. At somewhat stronger fields the curves separate again due to the finite final kinetic energy. From the ϵ^2 dependence of the cc - aa coupling it is finally clear that the corresponding rate falls off as B^{-4} .

At strong fields the dipolar transitions show a similar classification. The 11 strongest ones do not need a proton spin flip but only a single or double electron spin flip. As a consequence the transitions are almost entirely due to $V^{d,ee}$. The spin matrix element is more or less independent of B (for strong fields). The highest category (7,8,12) consists of electron double spin-flip transitions. The middle category (9,13,16,17) of electron single spin-flip processes with $S=1$ in both initial and final states. The lowest category (10,11,14,15) comprises electron single spin-flip processes where the initial or final states have $S=1$ with only 50% probability. This reduces G by a factor of 2. The spin matrix element for the highest category differs by a factor $\sqrt{2}$ from that for the middle category. This is to be combined with a factor $\sqrt{2}$ from the phase-space factor $p_{\alpha\beta}$ in Eq. (34). The proportionality of the G values is clearly seen in Fig. 1(a). The initial gradual increase with B is due to the same factor $p_{\alpha\beta} \sim \sqrt{B}$. The explanation for the bending down of the curves at the highest B values is similar as for that of curves 1 and 6 considered before: the disparity in initial and final kinetic energies. It is clear that the highest category starts to bend down at smaller B : the double spin-flip energy is a factor of 2 larger.

The remaining dipolar rates all show a decreasing slope due to ϵ and ϵ^2 dependences of the electron-electron spin matrix element: The dominant initial and final proton

spin configurations are orthogonal. Hyperfine induced admixtures in one and two atoms, respectively, are required to achieve equal proton spin wave functions. The first category contains the $bb \rightarrow ab$ and $ab \rightarrow aa$ relaxations as special cases, and also $dd \rightarrow ac$, which is one of the most important dipolar transitions for the decay of the static magnetic trap. At the fields considered the electron-electron contribution dominates. At the higher fields electron-proton relaxation starts to take over. Depending on the relative sign of the electron-electron and electron-proton matrix elements, G curves start to bend down or up relative to their above-mentioned dominant slope.

V. CONCLUSIONS

Given the effective Hamiltonian the coupled-channels method is a rigorous method for calculating H+H spin-exchange and dipolar rates. In the foregoing we have described this method and some of its results: the B dependence of all $T=0$ rates and the T dependence of some $B=0$ rates. The latter have been selected on the basis of their importance for the cryogenic H maser and for the H1 magnetic trap. Closed-form formulas for the rates, useful for the analysis of both types of experiments, have been presented for the field and temperature dependence in the weak-field regime ($B \leq 0.1$ T), based on the degenerate-internal-states approximation. A simple interpretation has been given also for the strong-field behavior ($B \geq 1$ T) of the rates.

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CHAPTER 3:
TRAPPING OF NEUTRAL ATOMS
WITH RESONANT MICROWAVE RADIATION

Trapping of Neutral Atoms with Resonant Microwave Radiation

Charles C. Agosta and Isaac F. Silvera

Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138

H. T. C. Stoof and B. J. Verhaar

Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

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We discuss a resonant microwave trap for neutral atoms. Because of the long spontaneous radiation time this trap is remarkably different from the optical trap. It also has advantages over static magnetic traps that trap the excited spin state of the lowest electronic level, in that atoms predominantly in the spin ground state can be trapped. We analyze the relaxation-ejection lifetime of atoms in such a trap using the formalism of dressed atomic states. Results are applied to atomic hydrogen and the possibility of Bose-Einstein condensation is considered.

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The past several years have been witness to the exciting development of trapping of neutral atoms with optical radiation from a laser source¹ or with static magnetic fields.²⁻⁴ In this Letter we show that a gas of atoms can be trapped using forces derived from the gradient of a microwave radiation field on resonance with an atomic transition.⁵ The principal difference between microwave and optical traps is the virtual absence of microwave spontaneous emission. This changes the nature of the trap potential and eliminates the spontaneous emission heating of the atoms. In comparison to the static magnetic trap the microwave trap has the primary advantage of being able to trap atoms with a ground-state character. Because the static magnetic trap utilizes a field minimum,⁶ it is limited to trapping of atoms in the ground electronic state with excited spin states, which spin relax to the ground state at a density-dependent rate. These lower-state atoms are then ejected from the trap,⁷ resulting in low densities of trapped atoms. In contrast, the microwave trap can operate with either a field maximum or minimum and the trapped atoms will be an admixture of the excited and the ground states, depending on the detuning of the radiation from resonance. We study the lifetime of the atomic density and show that it can be much longer in a microwave trap than in the static trap and thus much higher densities are possible. This is important in efforts to obtain Bose-Einstein condensation (BEC) in atomic hydrogen, which is discussed as a specific example.

We first derive the trap potential.⁸ We shall treat the atom as a two-level system and denote the states $|e\rangle$ and $|g\rangle$ for excited and ground states. A very simple approach for calculating the depth of a magnetic trap is the dressed-atom approach used for optical traps by Dalibard and Cohen-Tannoudji.^{9,10} An atom in a single-mode radiation field with magnetic operator \mathbf{B}_R can be described by the following Hamiltonian,

$$\mathcal{H} = H_R + H_{\text{atom}} - \mu \cdot \mathbf{B}_R(\mathbf{r}). \quad (1)$$

Here, $H_R = \hbar \omega a^\dagger a$ is the Hamiltonian of the radiation

field with photon angular frequency ω and creation and annihilation operators a^\dagger and a , respectively. $H_{\text{atom}} = p^2/2m + \hbar \omega_0 b^\dagger b$ is the Hamiltonian of the atom of mass m with the two levels separated in energy by $\hbar \omega_0$, where b^\dagger and b are the atomic raising and lowering operators for the levels $|e\rangle$ and $|g\rangle$. We have assumed that the atom interacts with a magnetic field $\mathbf{B} = \mathbf{B}_0 + \mathbf{B}_R$ through its magnetic dipole moment μ . \mathbf{B}_0 is a static field and is included in H_{atom} . If there is no zero-field splitting of the atom, the resonance frequency is $\omega_0 = \mu_B B_0 / \hbar$, where μ_B is the Bohr magneton. The last term in Eq. (1) is the interaction of the atom with the microwave field which, including resonant terms only, is given by $-\mu_{eg} \cdot \lambda \mathcal{B}(\mathbf{r})(a^\dagger b + ab^\dagger)$, where μ_{eg} is a magnetic dipole transition-matrix element and λ is the polarization vector.

If the interaction between the field and the atom is zero then the eigenstates of this Hamiltonian fall into manifolds separated by energy $\hbar \omega$. Each manifold consists of a pair of states $|g, N\rangle$ and $|e, N-1\rangle$ split by $\hbar \delta$, where N is the photon occupation number and $\delta = \omega - \omega_0$ is the detuning. When the coupling term is included, the dressed states are⁹

$$|1N\rangle \equiv |1\rangle = \cos\theta(\mathbf{r}) |e, N-1\rangle + \sin\theta(\mathbf{r}) |g, N\rangle, \quad (2a)$$

$$|2N\rangle \equiv |2\rangle = -\sin\theta(\mathbf{r}) |e, N-1\rangle + \cos\theta(\mathbf{r}) |g, N\rangle, \quad (2b)$$

where the angle $\theta(\mathbf{r})$ is defined by $\cos 2\theta(\mathbf{r}) = -\delta/\Omega(\mathbf{r})$ and $\sin 2\theta(\mathbf{r}) = \omega_r(\mathbf{r})/\Omega(\mathbf{r})$. Here, $\omega_r = \mu_{eg} \cdot \lambda 2\sqrt{N} \times \mathcal{B}(\mathbf{r})/\hbar$ is the Rabi frequency, and $\Omega(\mathbf{r}) = [\omega_r^2(\mathbf{r}) + \delta^2]^{1/2}$. The corresponding energies are $E_{iN}(\mathbf{r}) = N\hbar\omega + E_i(\mathbf{r})$ with

$$E_1(\mathbf{r}) = -\hbar\delta/2 + \hbar\Omega(\mathbf{r})/2, \quad (3a)$$

$$E_2(\mathbf{r}) = -\hbar\delta/2 - \hbar\Omega(\mathbf{r})/2. \quad (3b)$$

These energy levels vary with position in an inhomogeneous field through the dependence of the Rabi frequency on \mathbf{r} .

The depth of the trap is the difference in energy for an atom in the microwave field and its energy in zero field.

For a microwave field with a maximum, state $|2\rangle$ is a trapping state with potential

$$U_i = \hbar/2[|\delta| - (\omega_r^2 + \delta^2)^{1/2}]. \quad (4)$$

State $|1\rangle$ is a barrier state or an antitrapping state with $U_{at} = -U_i$. The maximum trap depth is at $\delta=0$, yielding $U_{i\max}/k_B = \hbar\omega_r/2k_B = 0.47B_R$ in kelvins with B_R in teslas. Here we have taken $\mu_{eg} \cdot \lambda = \sqrt{2}\mu_B$ and have used circularly polarized microwave radiation; for linearly polarized radiation the depth is reduced by $\sqrt{2}$. The microwave trap has the interesting property that U_i has its maximum depth for $\delta=0$ and $|2\rangle$ remains a trapping state for both positive and negative values of δ . Moreover, as can be seen from the states in Eq. (2b), the nature of $|2\rangle$ changes from predominantly $|e, N-1\rangle$ to $|g, N\rangle$ as δ goes from positive to negative values. In Figs. 1(a) and 1(b), we plot the trap potential for the two dressed states as a function of the detuning δ , as well as the dependence of the admixture of states on detuning.

We contrast these results with the optical laser trap where the excited state is separated from the ground state by an optical interval. This has a potential well^{9,11}

$$U_{\text{opt}} = (\hbar/2)\delta \ln(1 + \omega_r^2/2\delta^2), \quad (5)$$

also plotted in Fig. 1(a) for the same interaction as in Eq. (1). In this trap $U_{\text{opt}}=0$ for $\delta=0$ and the potential changes from trapping to antitrapping as δ changes sign. This remarkable change of nature from the microwave case is caused by the short spontaneous emission lifetime characteristic of electric dipoles in the optical region (of order 10^{-8} s) which couple the dressed manifolds. By contrast, electron-spin magnetic dipole transitions have spontaneous-emission lifetimes of several million years. In an optical trap, an atom makes many transitions between dressed states in the time required to move across the trap and the force is an average found by multiplying the time spent in each state times the force in each state, resulting in Eq. (5). For $\delta=0$ the dressed states are equal admixtures of $|e, N-1\rangle$ and $|g, N\rangle$ so that the time spent in each state is equal, thus the force is zero. In the microwave case there is virtually no spontaneous emission; in addition it is easy to show that nonadiabatic transition rates are negligible. For these reasons the states of the atoms remain unchanged in time. This results in a deeper potential as a function of δ [see Fig. 1(a)]; it also precludes spontaneous emission heating which plagues the optical trap. Still, to create a useful well depth, large-amplitude microwave fields are needed. They can be attained in a cavity such as a concentric resonator; the application of such a resonator to the microwave trap has been discussed elsewhere.⁸

Unlike the above traps, the static magnetic trap, which has a depth $|U_i| = |\mu_B \Delta B_0|$, can be made much deeper with a large static gradient ΔB_0 on the order of 1 T. However, the trapped atoms must be in state $|e\rangle$ since a

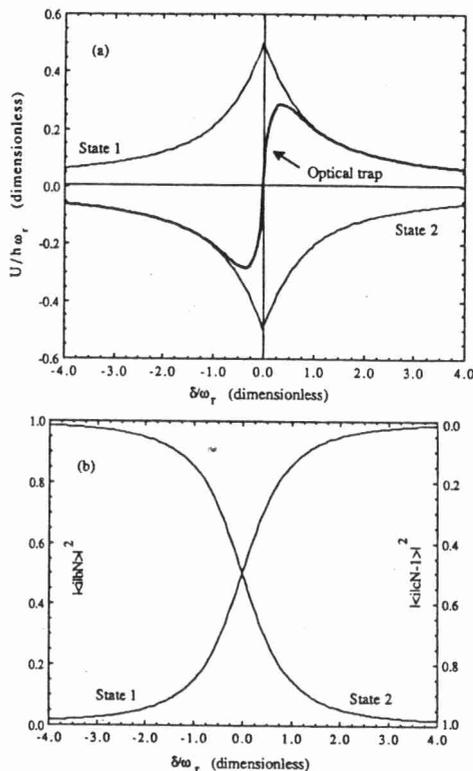


FIG. 1. (a) Potential depth for the two dressed atom states compared to the depth for an optical trap (with the same interaction) as a function of δ/ω_r . (b) The probabilities for the bare states as admixed into the trapping and antitrapping states, as a function of δ/ω_r .

static trap can only be made with a field maximum. Because of density-dependent collisional relaxation to state $|g\rangle$, which is an antitrapping state (atoms are ejected), the density in this trap rapidly decays down to a relatively low value.

A crucial consideration of the viability of the microwave trap is its lifetime for decay of the density due to collisional relaxation. Although this trap can be applied to any species with an effective two-level system, we shall consider atomic hydrogen, and compare it to the existing static trap. Hydrogen has four hyperfine states enumerated $|a\rangle$, $|b\rangle$, $|c\rangle$, and $|d\rangle$, from low to high energy. In a high field, electron-spin resonance is allowed between states $|b\rangle$ and $|c\rangle$ (as well as $|a\rangle$ and $|d\rangle$). We shall focus on the $|b\rangle$ and $|c\rangle$ states as a two-level

system, modifying our earlier notations so that $|g\rangle \equiv |b\rangle$ and $|e\rangle \equiv |c\rangle$. Since the dressed state $|2\rangle$ is an admixture of $|b\rangle$ and $|c\rangle$, $|2\rangle$ - $|2\rangle$ binary collisions can result in the transition of $|c\rangle$ to $|b\rangle$ during a collision. A transition to a b state results in the formation of state $|1\rangle$ or $|2\rangle$ with a calculable probability. Since those atoms in state $|1\rangle$ are ejected, the density decays. Collisional relaxation between bare states $|b\rangle$ and $|c\rangle$ have been studied earlier⁷ and are a result of spin-exchange or magnetic dipole-dipole interactions. Both T_1 (inelastic relaxation) and T_2 (dephasing of the transverse spin) processes can lead to decay of the density of atoms in state $|2\rangle$. We find that the T_1 processes correspond to relaxation between dressed-atom manifolds, whereas the T_2 processes occur within a single manifold and have the unusual property of being thermally activated. This can be understood by considering states $|2\rangle$ and $|1\rangle$ in the rotating coordinate system of the rf magnetic field. An

isolated atom in the state $|2\rangle$ has its fictitious spin $\frac{1}{2}$ pointing along the effective field, whereas $|1\rangle$ points opposite. A T_2 collision will shift the transverse component of the spin leading to a superposition of states $|1\rangle$ and $|2\rangle$ and thus to decay by ejection. In a preliminary consideration of relaxation in the microwave trap,⁸ T_2 events were not considered and some coherent contributions to T_1 were omitted. Here we consider both channels of relaxation using a T -matrix formalism [Eq. (7), below]. Our detailed considerations will be focused on hydrogen, but the concepts are applicable to other species such as sodium, and we shall first present a general treatment.

Outside the range of the interatomic interaction two bare atoms interact only with the radiation field. In this situation the combined system of photons and atoms can be described by the symmetrized and normalized states $|ij\rangle N$:

$$\begin{aligned} |11\rangle N &= \cos^2\theta |ee\rangle, N-2 + (1/\sqrt{2}) \sin 2\theta |eg\rangle, N-1 + \sin^2\theta |gg\rangle, N, \\ |12\rangle N &= -(1/\sqrt{2}) \sin 2\theta |ee\rangle, N-2 + \cos 2\theta |eg\rangle, N-1 + (1/\sqrt{2}) \sin 2\theta |gg\rangle, N, \\ |22\rangle N &= \sin^2\theta |ee\rangle, N-2 - (1/\sqrt{2}) \sin 2\theta |eg\rangle, N-1 + \cos^2\theta |gg\rangle, N. \end{aligned} \quad (6)$$

The energies are $E_{ijN} = N\hbar\omega + E_i + E_j$ [cf. Eq. (3)]. These states may be interpreted as the free states of two indistinguishable dressed atoms and correspond to the possible initial and final channels of a scattering process.¹² The relaxation rates for the processes $ijN \rightarrow i'j'N'$ are found from a T -matrix calculation¹³

$$G_{ijN \rightarrow i'j'N'}(T) = 4\pi^2 \hbar^2 \mu \left\langle p_{i'j'} \sum_{l'm} |T_{l'm} i'j'N', l'm | ij\rangle N (p_{i'j'}, p_{ij}) \right\rangle_{th}^2, \quad (7)$$

where μ is the reduced mass, p_{ij} and $p_{i'j'}$ are the magnitude of the initial and final relative momenta, respectively, and the subscript th implies a thermal average. Note that to find the decay of the atomic density inside the trap we should, in addition to the thermal average over initial momenta p_{ij} , average over the number of photons. However, in an intense radiation field we can neglect fluctuations and replace N by its average value \bar{N} in Eq. (7). The relevant decay rates are then $G_{22\bar{N} \rightarrow i'j'N'}(T)$.

To evaluate these quantities it is important to point out that the central (singlet or triplet) interaction between two bare hydrogen atoms couples only the states $|ij\rangle N$ with the same value of N . Since the energy splitting $\hbar\Omega$ within this manifold is very small compared to the strength of the central interaction, the degenerate-internal-states (DIS) approximation¹³ is valid and used throughout the following. Note that the dipolar

transitions among states with the same N are completely suppressed by the centrifugal barrier in either the initial or final state.

If $N' = \bar{N}$ all processes are endothermic. In order to find the dominant low-temperature behavior of the rates we use the relation¹³

$$G_{22\bar{N} \rightarrow i'j'N'}(T) = G_{i'j'N' \rightarrow 22\bar{N}}(T) \exp(-\Delta_{i'j'}/k_B T), \quad (8)$$

expand the rate constant for the inverse (exothermic) reaction, and take the lowest order $k_B T/\Delta_{i'j'}$, where $\Delta_{i'j'} = \hbar\Omega(\delta_{i',1} + \delta_{j',1})$ denotes the energy difference between the final and initial channels. This expansion is found by applying the DIS approximation to the T matrix in Eq. (7). Doing so, we find that transitions within a manifold are associated with elastic exchange collisions between bare atoms and are at an effective rate defined by $dn/dt = -G_{i'j'N'}^{\text{eff}} n^2$. For the hydrogen atom

$$G_{i'j'N'}^{\text{eff}} = 2.3 \times 10^{-13} (\hbar\Omega/k_B)^{1/2} \sin^2 2\theta [B_C^2 / (B_C^2 + B_C^2)] [\sin^4 \theta \exp(-\hbar\Omega/k_B T) + \sqrt{2} \exp(-2\hbar\Omega/k_B T)] \quad (9)$$

in units of cm^3/s with the static field B_0 in tesla and the constant $B_C = 0.05064$ T originating from a consideration of the hyperfine levels in the field B_0 .

To obtain the above expression, one has to evaluate the difference $T_{00[\text{cc}],00[\text{cc}]}(0,0) - T_{01}(0,0)$, where $T_{ij}(0,0)$ is a (on-shell) T -matrix element for singlet or triplet scattering at zero energy. Applying the DIS approximation once again, but now to bare atom states, this difference can be expressed in terms of scattering lengths $a^{(i)}$. In this second DIS approximation, we assume the hyperfine states $|\text{cc}\rangle$, $|\text{bd}\rangle$, $|\text{ac}\rangle$, and $|\text{aa}\rangle$ to be degenerate, similar to the

same assumption for the dressed states $|ij\rangle N$ within a manifold. The result is

$$T_{00|cc\rangle,00|cc\rangle}(0,0) - T_{01}(0,0) \\ = [B\tilde{\chi}/(B\tilde{\chi}_0 + B\tilde{\chi})](2\pi\hbar m_H)^{-1}(a^{(0)} - a^{(1)}). \quad (10)$$

Equation (10) is fully confirmed by a rigorous coupled-channel calculation. A numerical evaluation of Eq. (9) shows that in the experimental circumstances envisaged, i.e., strong magnetic fields of order 5 T, the T_2 processes are unimportant compared to (T_1) transitions between different manifolds which are due mainly to dipolar interactions and will be considered next.

Dipolar relaxation caused by the dominant electron-electron magnetic interaction V^d is possible for both $N' = \bar{N} - 1$ and $\bar{N} - 2$. Because this weak interaction can be treated as a small perturbation, we have

$$T_{r'm'|i'j'N',lm|ijN}(p_{r'j'}, p_{ij}) \\ = \langle \psi_{r'm'|i'j'N'}^- | V^d | \psi_{lm|ijN}^+ \rangle_c, \quad (11)$$

using the notation of Ref. 13. The initial and final distorted wave functions incorporate the central interaction to all orders and can be approximated by neglecting the energy splitting within the respective manifolds $|ij\rangle N$ and $|i'j'\rangle N'$. Furthermore, if we make use of the fact that at high magnetic fields the hyperfine state $|cc\rangle$ has a dominant triplet character, we get

$$G_{T_1}^{\text{eff}}(B, T) = \sin^4\theta[4\sin^2 2\theta + (1 - 4\cos^2\theta)^2]G_{cc \rightarrow bc}(B, T) + 2\sin^4\theta(\sin^4\theta + \frac{1}{4}\sin^2 2\theta)G_{cc \rightarrow bb}(B, T). \quad (12)$$

Here $G_{T_1}^{\text{eff}}$ is defined locally by $dn_1/dt = -G_{T_1}^{\text{eff}}n_1^2$.

Because of the phase relations between interfering T -matrix elements, the rate (12) could be expressed in the rates $G_{cc \rightarrow bc}$ ($= G_{bc \rightarrow bb}$) and $G_{cc \rightarrow bb}$ for collisions between bare hydrogen atoms, which have been calculated previously in Refs. 7 and 13. Note that from these papers we find a justification for the neglect of the $|a\rangle$ and $|d\rangle$ hyperfine states in the above treatment. At magnetic field strengths of the order of 5 T, the dominant relaxation processes in a gas of atoms populating the b and c states are $cc \rightarrow bb$, $cc \rightarrow bc$, and $bc \rightarrow bb$. From these results we find that the half-life of the trapped atoms is $\tau = (G_{T_1}^{\text{eff}}n_0)^{-1}$, where n_0 is the initial trapped density. In Fig. 2 we plot $G_{T_1}^{\text{eff}}$ as a function of θ , as well as G^{eff} for the static trap.⁷ We see that by detuning to small θ so that $|2\rangle = |g, N\rangle$ the microwave trap can be made much more stable than the static trap. The resulting potentially higher starting densities overcome the difficulties of attaining BEC, addressed by Tommila.¹⁴ Evaporative cooling¹⁵ of the trapped atoms as a means of attaining BEC can be easily accomplished by detuning, which lowers the well depth.

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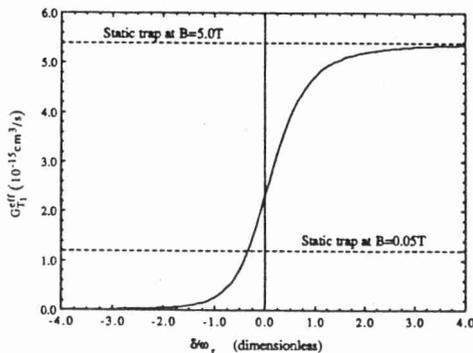


FIG. 2. Decay-rate constant of hydrogen atoms in the microwave trap as a function of δ/ω_r . We compare to the static trap for magnetic fields of 0.05 and 5 T.

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CHAPTER 4:
DECAY OF SPIN-POLARIZED ATOMIC HYDROGEN
IN THE PRESENCE OF A BOSE CONDENSATE

Decay of spin-polarized atomic hydrogen in the presence of a Bose condensate

H. T. C. Stoof, A. M. L. Janssen, J. M. V. A. Koelman, and B. J. Verhaar

Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

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We study the decay of magnetically trapped doubly spin-polarized atomic hydrogen in the density and temperature regime of the Bose-Einstein phase transition and calculate the temperature and magnetic field dependence of all relevant relaxation rate constants $G_{dd \rightarrow \kappa\lambda}$. At the transition temperature T_c the rate constants have a discontinuous second derivative with respect to T . Below T_c they show a pronounced decrease relative to the extrapolated above- T_c values, the observation of which is a clear signal for the experimental realization of Bose-Einstein condensation.

I. INTRODUCTION

The possibility of trapping and subsequent cooling of neutral atoms down to temperatures in the range of 1–100 μK has given rise to the opportunity, at least in principle, to study the behavior of ultracold gases in the low-temperature and high-density regime where collective quantum effects due to degeneracy are expected to show up. The first experiments in this context used sodium atoms and a magnetic¹ or optical² trap. However, in the cases the achieved densities were far too low to observe any deviations from classical statistics.

From the point of view of achieving the Bose-Einstein transition, magnetically trapped doubly spin-polarized atomic hydrogen ($\text{H}\uparrow\uparrow$) seems to be much more promising,³ primarily since its atomic mass is much smaller and the attractive well due to the van der Waals interaction between the atoms is very shallow. At temperatures of the order of 10 μK the required densities are so low that only two-body collisions affect the decay of the gas. Hence the three-body recombination process which dominates in the compression experiments with $\text{H}\uparrow\uparrow$ in liquid-helium-covered sample cells^{4,5} is avoided.

Recently Hess *et al.*⁶ and van Roijen *et al.*⁷ reported on the successful trapping of hydrogen atoms at temperatures of about 1 and 100 mK, respectively. A very good quantitative agreement was found with our theoretical predictions⁸ for the decay of the gas, both with respect to the magnitude⁶ and the magnetic field and temperature dependence.⁷ However, these calculations assume a Maxwell-Boltzmann velocity distribution in the gas and thus apply only to the nondegenerate regime in which the above-mentioned experiments are carried out. In this paper we will relax this condition and study the dominant relaxation processes in $\text{H}\uparrow\uparrow$ in a wide temperature range and especially at temperatures below the critical temperature T_c .

To this end we consider in Sec. II the eigenstates of N weakly interacting hydrogen atoms with (electron and proton) spin degrees of freedom by an extension of the ξ method developed by Lee and Yang.⁹ We derive the free energy of the system from which all thermodynamical equilibrium quantities, and in particular the condensate fraction for the $|\uparrow\uparrow\rangle$ spin state, can be found. In Sec. III

we use this formalism to calculate all electron-electron dipolar decay rates $G_{dd \rightarrow \kappa\lambda}$ (the hyperfine states of the 1s ground state of atomic hydrogen are denoted by $|a\rangle$, $|b\rangle$, $|c\rangle$, and $|d\rangle$ in order of increasing energy) as a function of T and applied magnetic field B and compare with results obtained earlier. We will also show that the dominant temperature dependence for sufficiently exothermic reactions can be found by an extension of the correlator discussed by Kagan *et al.*¹⁰ to the case of two-body relaxation processes. Section IV will give some concluding remarks.

II. ATOMIC HYDROGEN AS A WEAKLY INTERACTING BOSE GAS

We consider a homogeneous system of N hydrogen atoms with internal degrees of freedom corresponding to the hyperfine states $|\alpha\rangle$ and the energy eigenvalues ϵ_α . In addition, we use a quantization volume V and periodic boundary condition to facilitate the treatment of the condensate. Our final results will be presented in the thermodynamical limit ($N, V \rightarrow \infty$ and $n = N/V$ constant). The normalized and discrete one-atom states with momentum $\hbar\mathbf{k}$ are denoted by $|\mathbf{k}\alpha\rangle$ and have an energy

$$\epsilon_{\mathbf{k}\alpha}^0 = \frac{\hbar^2 \mathbf{k}^2}{2m_H} + \epsilon_\alpha, \quad (1)$$

where m_H is the mass of the hydrogen atom.

The phenomenon of Bose-Einstein condensation in the case of magnetically trapped atomic hydrogen is associated with a macroscopic occupation of the state $|0d\rangle$. Although $|0d\rangle$ is not the one-atom ground state the condensation occurs into this state, because of a spontaneously developing nonequilibrium situation in spin space: Only the doubly polarized $|d\rangle = |\uparrow\uparrow\rangle$ state remains populated, since the "high-field seeking" a and b atoms are not trapped in a minimum B field, while the "low-field seeking" c atoms are rapidly removed from the trap due to exchange relaxation processes.^{11,8}

The details of the macroscopic occupation depend to a great extent on the interaction between the particles. In the following we show that the deviations from the ideal Bose gas are characterized by the parameters $(na^3)^{1/4}$, $(na\Lambda^2)^{1/2}$ and their ratio $(a/n\Lambda^4)^{1/4}$. Here a is the (trip-

let) scattering length which characterizes the strength of the interaction and Λ denotes the thermal de Broglie wavelength

$$\Lambda(T) = \left[\frac{2\pi\hbar^2}{m_H k_B T} \right]^{1/2}, \quad (2)$$

with k_B Boltzmann's constant. For atomic hydrogen with a density of 10^{14} cm^{-3} and a temperature equal to the critical temperature $T_c \approx 34 \mu\text{K}$ these parameters are small. We therefore neglect first and higher orders in these parameters but take all orders of the degeneracy parameter $n\Lambda^3$ into account, since we want to consider the regime where Bose-Einstein condensation takes place ($n\Lambda^3 \approx 1$).

The decay of the fully (doubly) polarized gas is due to the weak electron-electron dipolar interaction, which can be treated as a perturbation. This section is concerned with the associated "zeroth-order" problem, in which the central (singlet or triplet) interaction is taken into account. In Sec. III we then turn to the influence of the dipolar interaction.

A. Hamiltonian and eigenstates

At the low temperatures ($a/\Lambda \ll 1$) in which we are interested, it is permitted to use the pseudopotential method¹² and replace the real potential $V_{\alpha'\beta, \alpha\beta}(r)$, which depends on the internal states involved in the interaction, by a pseudopotential $v_{\alpha'\beta, \alpha\beta}\delta(r)$ with the same scattering properties for low energies. This requires $v_{\alpha'\beta, \alpha\beta}$ to be equal to an (on-shell) two-body T -matrix¹³ element at zero energy, which in turn can be expressed in singlet and triplet scattering lengths $a^{(S)}$ if we use the very accurate "degenerate-internal-states" approximation.⁸ Denoting the projection operators on the part of spin space with total electron spin equal to S by $\mathcal{P}^{(S)}$, the result is given by

$$v_{\alpha'\beta, \alpha\beta} = \frac{4\pi\hbar^2}{m_H} \left\langle \alpha'\beta' \left| \sum_S a^{(S)\mathcal{P}^{(S)}} \right| \alpha\beta \right\rangle. \quad (3)$$

In particular, the important quantity $v_{dd, dd}$ is equal to $4\pi\hbar^2 a^{(1)}/m_H \equiv 4\pi\hbar^2 a/m_H$.

In second quantization and with the convenient notation $v_{\alpha'\beta, \alpha\beta}^{id} = v_{\alpha'\beta, \alpha\beta} + v_{\alpha'\beta, \beta\alpha}$ the Hamiltonian of the system takes the form

$$H = \sum_{\alpha} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}\alpha}^0 a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} + \frac{1}{4V} \sum_{\alpha\beta\alpha'\beta'} v_{\alpha'\beta, \alpha\beta}^{id} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a_{\mathbf{k}+\mathbf{q}\alpha}^\dagger a_{\mathbf{k}'-\mathbf{q}\beta} a_{\mathbf{k}\alpha} a_{\mathbf{k}'\beta}, \quad (4)$$

with the creation (annihilation) operators $a_{\mathbf{k}\alpha}^\dagger$ ($a_{\mathbf{k}\alpha}$) obeying the usual commutation relations. Following the discussion by Lee and Yang⁹ for a population of the $|Od\rangle$ state by a finite fraction ξ of the total number of particles N , we consider a free state $|\{N_{\mathbf{k}\alpha}^0\}\rangle$ with a set of occupation numbers such that

$$\begin{aligned} N_{Od}^0 &= \xi N, \\ N_{\mathbf{k}d}^0 &= O \left[\frac{N^{1/3} (na^3)^{1/6}}{na\Lambda^2} \right] \text{ if } \mathbf{k} \neq 0, \\ N_{\mathbf{k}\alpha}^0 &= O(1) \text{ if } \alpha \neq d, \end{aligned} \quad (5)$$

and

$$\sum_{\mathbf{k} \neq 0} N_{\mathbf{k}d}^0 + \sum_{\alpha \neq d} \sum_{\mathbf{k}} N_{\mathbf{k}\alpha}^0 = (1 - \xi) N. \quad (6)$$

The last line of Eq. (5) reflects the nonequilibrium situation in spin space as mentioned previously: A gas of d atoms can only decay by dipolar relaxation and produce atoms in an $|a\rangle$, $|b\rangle$, or $|c\rangle$ state, which are then rapidly removed from the trapping region.

Including the interaction the free state $|\{N_{\mathbf{k}\alpha}^0\}\rangle$ will evolve into a state of $\{N_{\mathbf{k}\alpha}^0\}$ quasiparticles which can be seen as a superposition of free states with occupation numbers $N_{\mathbf{k}\alpha}$ differing from $N_{\mathbf{k}\alpha}^0$ by $\delta_{\mathbf{k}\alpha}$:

$$N_{\mathbf{k}\alpha} = N_{\mathbf{k}\alpha}^0 + \delta_{\mathbf{k}\alpha}. \quad (7)$$

A posteriori it is possible to show that the expectation value of $\delta_{\mathbf{k}\alpha}$ in the resulting state of quasiparticles obeys

$$\langle \delta_{\mathbf{k}d} \rangle = O \left[\frac{N^{2/3} (na^3)^{1/3}}{na\Lambda^2} \right] \text{ if } \mathbf{k} \neq 0, \quad (8)$$

$$\langle \delta_{\mathbf{k}\alpha} \rangle = 0 \text{ if } \alpha \neq d,$$

while the fluctuations of the condensate fraction satisfy

$$\left\langle \left(\frac{1}{N} \sum_{\mathbf{k} \neq 0} \delta_{\mathbf{k}d} \right)^2 \right\rangle = O \left[\frac{(na^3)^{1/2}}{na\Lambda^2} \right]. \quad (9)$$

From these estimates and the selection rule $\Delta M_F = 0$ for the central interaction, implying that

$$v_{dd, \alpha\beta}^{id} = v_{\alpha\beta, dd}^{id} = v_{dd, dd}^{id} \delta_{\alpha d} \delta_{\beta d}$$

and

$$v_{\alpha d, \beta d}^{id} = v_{dd, \alpha d}^{id} \delta_{\alpha\beta},$$

we find that the only terms in the Hamiltonian contributing in the thermodynamical limit are

$$\begin{aligned} H &= \sum_{\alpha} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}\alpha}^0 a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} + \frac{v_{dd, dd}^{id}}{4V} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a_{\mathbf{k}+\mathbf{q}d}^\dagger a_{\mathbf{k}'-\mathbf{q}d} a_{\mathbf{k}d} a_{\mathbf{k}'d} \\ &+ \sum_{\alpha \neq d} \frac{v_{\alpha d, \alpha d}^{id}}{4V} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a_{\mathbf{k}+\mathbf{q}\alpha}^\dagger a_{\mathbf{k}'-\mathbf{q}\alpha} a_{\mathbf{k}\alpha} a_{\mathbf{k}'\alpha}. \end{aligned} \quad (10)$$

In the nondiagonal part of this Hamiltonian, coupling the single-particle states, we neglect all but the terms of highest order in the number of condensate particles and in view of Eq. (9) also the fluctuations of the condensate fraction. This leads to

$$H^{ND} \approx \frac{\xi n}{4} v_{dd, dd}^{id} \sum_{\mathbf{k} \neq 0} (a_{\mathbf{k}d}^\dagger a_{-\mathbf{k}d}^\dagger + a_{\mathbf{k}d} a_{-\mathbf{k}d}). \quad (11)$$

The diagonal part is rewritten in terms of the occupation numbers $N_{\mathbf{k}\alpha}$ with the result

$$H^D = \frac{v_{dd,dd}^{id}}{4V} \left[2 \left(\sum_{\mathbf{k}} N_{k d} \right)^2 - \sum_{\mathbf{k}} N_{k d}^2 - \sum_{\mathbf{k}} N_{k d} \right] + \sum_{\alpha \neq d} \frac{v_{\alpha d, \alpha d}^{id}}{V} \sum_{\mathbf{k}} \left(\sum_{\mathbf{k}'} N_{\mathbf{k}' d} \right) N_{\mathbf{k} \alpha} . \quad (12)$$

The last term reduces in thermodynamical limit to the

$$\frac{v_{dd,dd}^{id}}{4V} \left[N^2 [1 + (1 - \xi)^2] + 2\xi N \sum_{\mathbf{k} \neq 0} N_{k d} - 2(2 - \xi) N \sum_{\alpha \neq d} \sum_{\mathbf{k}} N_{k \alpha} \right] + W ,$$

where W equals

$$\frac{v_{dd,dd}^{id}}{4V} \left[-N - \sum_{\mathbf{k} \neq 0} N_{k d}^2 - \left(\sum_{\mathbf{k} \neq 0} \delta_{k d} \right)^2 + \sum_{\alpha \neq d} \sum_{\mathbf{k}} N_{k \alpha} + 2 \left(\sum_{\alpha \neq d} \sum_{\mathbf{k}} N_{k \alpha} \right)^2 \right] .$$

This contribution can be neglected since explicit calculation shows that in addition to Eq. (9) we have

$$\sum_{\mathbf{k} \neq 0} \langle N_{k d}^2 \rangle = O \left[\frac{N^{4/3} (na^3)^{2/3}}{(na \Lambda^2)^2} \right] . \quad (13)$$

Therefore, in the thermodynamical limit, W leads to negligible corrections of order $N(na^3)^{1/2} k_B T$ to the energy eigenvalues (and thus the free energy).

Collecting the remaining results, we find that the Hamiltonian of the gas can be approximated to a high degree of accuracy by

$$H \simeq N [1 + (1 - \xi)^2] \frac{nv_{dd,dd}^{id}}{4} + \sum_{\mathbf{k} \neq 0} \left[\epsilon_{k d}^0 + \frac{\xi}{2} nv_{dd,dd}^{id} \right] a_{k d}^\dagger a_{k d} + \frac{\xi}{4} nv_{dd,dd}^{id} \sum_{\mathbf{k} \neq 0} \left[a_{k d}^\dagger a_{-k d}^\dagger + a_{k d} a_{-k d} \right] + \sum_{\alpha \neq d} \sum_{\mathbf{k}} \left[\epsilon_{k \alpha}^0 + nv_{\alpha d, \alpha d}^{id} - (1 - \xi/2) nv_{dd,dd}^{id} \right] a_{k \alpha}^\dagger a_{k \alpha} , \quad (14)$$

where we have taken ϵ_{0d}^0 as our zero-point of energy. This Hamiltonian can be diagonalized by means of a Bogoliubov transformation¹⁴ of the operators $a_{k d}^\dagger$ and $a_{k d}$ to creation ($b_{k d}^\dagger$) and annihilation ($b_{-k d}$) operators of $|d\rangle$ -state quasiparticles. To lowest order in $(na^3 \xi^2)^{1/2}$ the result is written as

$$H \equiv N [1 + (1 - \xi)^2] \frac{nv_{dd,dd}^{id}}{4} + \sum_{\mathbf{k} \neq 0} \epsilon_{k d} b_{k d}^\dagger b_{k d} + \sum_{\alpha \neq d} \sum_{\mathbf{k}} \epsilon_{k \alpha} a_{k \alpha}^\dagger a_{k \alpha} , \quad (15)$$

i.e., a Hamiltonian for a system of independent (quasi)particles with quasiparticle energies

$$\epsilon_{k d} = \epsilon_{k d}^0 \left[1 + \frac{n \xi v_{dd,dd}^{id}}{\epsilon_{k d}^0} \right]^{1/2} . \quad (16)$$

We remind the reader of the property that the dispersion relation is phononlike,

$$\epsilon_{k d} \simeq \hbar k (n \xi v_{dd,dd}^{id} / 2m_H)^{1/2} ,$$

for values of k small compared to $(na)^{1/2}$ and particlelike,

$$\epsilon_{k d} \simeq \epsilon_{k d}^0 + n \xi v_{dd,dd}^{id} / 2 ,$$

for $k \gg (na)^{1/2}$.

In the case of atomic hydrogen it is important to note that the densities and temperatures near the Bose-

Hartree-Fock correction to the energy of the α atoms due to the interaction with the total set of d atoms, i.e.,

$$\sum_{\alpha \neq d} \sum_{\mathbf{k}} nv_{\alpha d, \alpha d}^{id} N_{k \alpha} .$$

Furthermore, using Eqs. (5)–(7) the remaining part of H^D can be written as

Einstein transition are such that $na \Lambda^2$ is a small quantity. This means that the relevant thermal momenta are always large compared to $\hbar(na)^{1/2}$. Therefore the dispersion relation is well approximated by its particlelike limit. This approximation is identical with a Hartree-Fock or mean-field treatment of the gas, taking the macroscopic occupation of the one-atom $|0d\rangle$ state into account.¹⁵ Notwithstanding the validity of the particlelike limit in our circumstances, it is of interest to impose this limitation only in the final stage of calculating rate constants in Sec. II B: We then find more explicitly the region of applicability of the results.

B. Thermal average

The previous derivation allows us to calculate the transition probabilities Γ for the relaxation processes. To find the rate constants we need to perform a thermal average over the possible initial states, without $\alpha \neq d$ atoms, at a certain temperature. In principle this would imply a summation of the form

$$\frac{1}{Z} \sum_{\xi=0(1/N)!} \sum_{|N_{k d}^0|} e^{-\beta E(\xi, \{N_{k d}^0\})} \Gamma(\xi, \{N_{k d}^0\}) , \quad (17)$$

with $\beta = (k_B T)^{-1}$, $E(\xi, \{N_{k d}^0\}) \equiv E_0(\xi) + E_{sp}(\xi, \{N_{k d}^0\})$ the eigenvalues of the Hamiltonian (15) and the sum over states Z as a normalization factor. The prime in the second summation sign indicates that the summations

over ξ and $\{N_{kd}^0\}$ are not independent because the occupation numbers N_{kd}^0 correspond not only to the number of quasiparticles with momentum $\hbar\mathbf{k}$, but also to the number of (real) particles with the same momentum from which this state evolved by inclusion of the interaction. Therefore they must satisfy the condition

$$N_{qp} \equiv \sum_{\mathbf{k} \neq 0} N_{kd}^0 = (1 - \xi)N \tag{18}$$

for the total number of quasiparticles.

It turns out that thermal averages of the type (17) are conveniently carried out by deleting the subsidiary condition using a grand canonical ensemble with an associated chemical potential $\mu(\xi)$ and by limiting oneself to one "most probable" value $\bar{\xi}$ to ξ , depending on temperature.^{9,16}

In the thermodynamical limit $\mu(\xi)$ and the corresponding fugacity $\zeta(\xi) \equiv e^{\beta\mu(\xi)}$ follow from

$$(1 - \xi)n = \frac{1}{(2\pi)^3} \int d\mathbf{k} \frac{1}{\zeta^{-1}(\xi)e^{\beta\epsilon_{kd}(\xi)} - 1}, \tag{19}$$

while $\bar{\xi}$ is the value of ξ for which the free energy per particle

$$f(\xi, \zeta(\xi)) = \frac{E_0(\xi)}{N} + \frac{k_B T}{(2\pi)^3 n} \int d\mathbf{k} \ln[1 - \zeta(\xi)e^{-\beta\epsilon_{kd}(\xi)}] + (1 - \xi) \ln \zeta(\xi). \tag{20}$$

is minimal.

Since Eq. (19) is equivalent to $\partial f(\xi, \zeta)/\partial \zeta = 0$, we have

$$\frac{df(\xi, \zeta(\xi))}{d\xi} = \frac{\partial f(\xi, \zeta)}{\partial \xi} \Big|_{\zeta}. \tag{21}$$

Therefore, using the expressions in Ref. 9 and expanding both Eqs. (19) and (21) in powers of $(n\Lambda^2\xi)^{1/2}$ we obtain the coupled set of equations

$$\begin{aligned} (1 - \xi)n &= \Lambda^{-3}[g_{3/2}(\xi) + O((n\Lambda^2\xi)^{1/2})], \\ \frac{df(\xi, \zeta)}{d\xi} &= \Lambda^{-2}[-4\pi \ln(\xi) - O((n\Lambda^2\xi)^{1/2})], \end{aligned} \tag{22}$$

from which we can deduce $\bar{\xi}$ and $\bar{\zeta} \equiv \zeta(\bar{\xi})$. In Eq. (22) we made use of the well-known Bose functions $g_n(\xi)$ (Ref. 17) defined by

$$g_n(\xi) = \sum_{i=1}^{\infty} \frac{\xi^i}{i^n} = \frac{1}{\Gamma(n)} \int_0^{\infty} dy \frac{y^{n-1}}{\zeta^{-1}e^y - 1}. \tag{23}$$

Especially those with $n = 1, \frac{3}{2}, 2$, and $\frac{5}{2}$ play an important role in Sec. III and are shown in Fig. 1.

The solution of Eq. (22) is fundamentally different below and above a critical temperature T_c , deviating only slightly (for atomic hydrogen $\Lambda \simeq a$ would correspond to a temperature of about 600 K) from the critical temperature T_0 of an ideal Bose gas:

$$\begin{aligned} T_c &= T_0 \left[1 + O\left(\frac{a}{\Lambda}\right) \right], \\ T_0 &= \frac{2\pi\hbar^2}{m_H k_B} \left[\frac{n}{g_{3/2}(1)} \right]^{2/3} = \frac{2\pi\hbar^2}{m_H k_B} \left[\frac{n}{2.612} \right]^{2/3}. \end{aligned} \tag{24}$$

In the nondegenerate case $T > T_c$ the derivative $df/d\xi$ is always greater than zero and thus $f(\xi, \zeta(\xi))$ has a minimum on the ξ axis, i.e.,

$$\begin{aligned} \bar{\xi} &= 0, \\ n\Lambda^3 &= g_{3/2}(\bar{\xi}). \end{aligned} \tag{25}$$

However, in the degenerate case $T < T_c$ a solution of $df/d\xi = 0$ exists and $\bar{\xi}$ becomes different from zero. It turns out that $\bar{\xi}$ and $\bar{\zeta}$ now obey

$$\begin{aligned} (1 - \bar{\xi})n &= \Lambda^{-3}[g_{3/2}(1) - O((n\Lambda^2\bar{\xi})^{1/4}) \\ &\quad + O((n\Lambda^2\bar{\xi})^{1/2})], \\ \bar{\zeta} &= 1 - O((n\Lambda^2\bar{\xi})^{1/2}), \end{aligned} \tag{26}$$

because

$$g_{3/2}(\xi) \underset{\xi \rightarrow 1}{\sim} g_{3/2}(1) - 2\pi^{1/2}(1 - \xi)^{1/2}.$$

(Refs. 17 and 18).

Omitting the higher-order terms the solution of Eqs. (25) and (26) is shown in Fig. 2, in which we present $\bar{\xi}$ and $\bar{\zeta}$ as functions of T/T_c . In particular, we recover the well-known (ideal Bose gas) power law for the number of particles in the condensate:

$$N_{0d} = \bar{\xi}N \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right]. \tag{27}$$

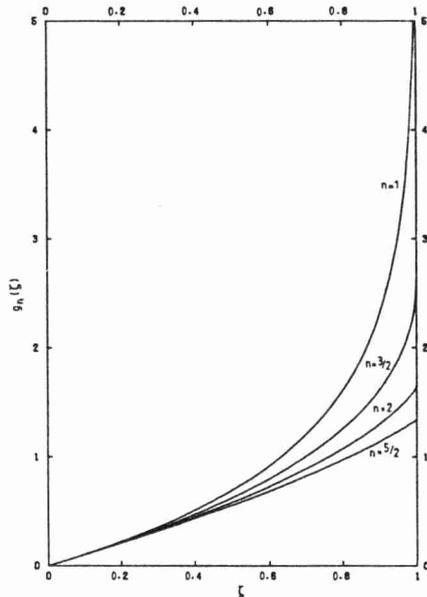


FIG. 1. Bose functions $g_n(\xi)$ for $n = 1, \frac{3}{2}, 2$, and $\frac{5}{2}$.

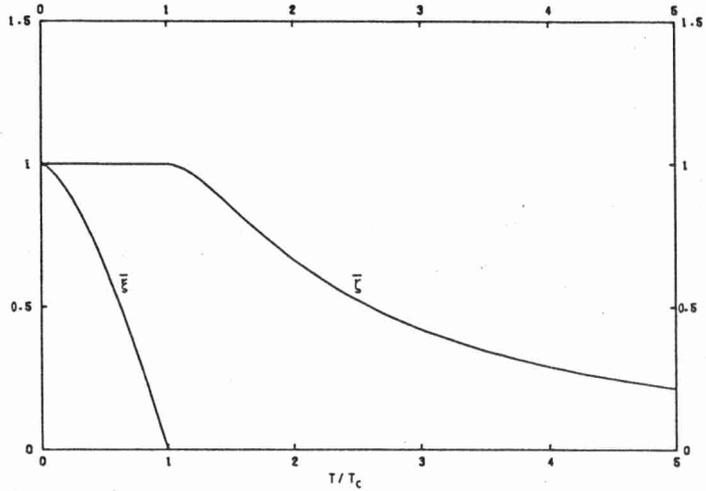


FIG. 2. Condensate fraction $\bar{\xi}$ and fugacity $\bar{\zeta}$ as functions of temperature.

Apparently, we find that a Bose gas behaves almost ideally if both $(na^3)^{1/4} \ll 1$ and $(na\Lambda^2)^{1/2} \ll 1$. However, as Eq. (9) explicitly shows, also the ratio of these parameters must be small compared to 1, for the $\bar{\xi}$ method to be self-consistent and the fluctuations of the condensate fraction to be negligible. This additional condition, which is not mentioned in Ref. 9, strongly restricts the region of applicability, but is still satisfied in the hydrogen case. Note that the smallness of $(a/n\Lambda^4)^{1/4}$ together with $(na^3)^{1/4} \ll 1$ implies $a/\Lambda \ll 1$.

The main conclusion of this section is that the thermal averages of the decay probabilities of interest can be carried out conveniently with a fixed- ξ ($=\bar{\xi}$) grand canonical ensemble. Although the summation over ξ has thus disappeared from Eq. (17), it is of importance to stress that this refers only to the initial states. A summation over final-state ξ values still occurs in the expression for the transition probability Γ . We come back to this in Sec. III.

III. DIPOLAR RELAXATION IN $H\uparrow\ddagger$

The dominant decay mechanism in $H\uparrow\ddagger$ is due to the magnetic dipolar interaction between the electron spins of the hydrogen atoms. This interaction is not invariant under spatial rotations and can be written as^{8,19}

$$V^d(\mathbf{r}) = -\frac{\mu_0\mu_e^2}{4\pi r^3} \left(\frac{4\pi}{5} \right)^{1/2} \sum_{\mu} Y_{2\mu}^*(\hat{\mathbf{r}}) \Sigma_{2\mu}^{ee}. \quad (28)$$

In terms of the total electron and proton spin states $|SM_S M_I\rangle$ the matrix elements of the tensor operator $\Sigma_{2\mu}^{ee}$ of rank 2 are proportional to a Clebsch-Gordan coefficient

$$\langle S'M_S I'M_I | \Sigma_{2\mu}^{ee} | SM_S IM_I \rangle = 2\sqrt{10} (SM_S 2\mu | S'M_S) \delta_{S,1} \delta_{S',1} \delta_{I,I'} \delta_{M_I, M_I'}, \quad (29)$$

from which the matrix elements in the basis $\{|\alpha\beta\rangle\}$ of hyperfine states can easily be calculated. We also need the Fourier transform of the spin matrix elements of $V^d(\mathbf{r})$:

$$V_{\alpha\beta', \alpha\beta}^d(\mathbf{q}) = \frac{\mu_0\mu_e^2}{3} \left(\frac{4\pi}{5} \right)^{1/2} \sum_{\mu} Y_{2\mu}^*(\hat{\mathbf{q}}) \langle \alpha'\beta' | \Sigma_{2\mu}^{ee} | \alpha\beta \rangle, \quad (30)$$

where the summation over μ reduces to only one term with μ equal to ΔM_F , i.e., the change of the total (electron) spin projection on the direction of the magnetic field.

As mentioned previously we treat the effect of the weak dipole interaction using first-order perturbation theory. The probability (per second) for a transition from a $|\xi_i, \{N_{kd}\}_i\rangle$ initial state of the doubly polarized gas to a final state $|\xi_f, \{N_{ka}\}_f\rangle$ with only one or two atoms having an internal state different from $|d\rangle$ obeys Fermi's golden rule,

$$\Gamma_{d \rightarrow \kappa i}(\xi_i, \{N_{kd}\}_i) = \frac{2\pi}{\hbar} \sum_{\xi_f} \sum_{\{N_{ka}\}_f} \delta''(E(\xi_f, \{N_{ka}\}_f) - E(\xi_i, \{N_{kd}\}_i)) \left| \langle \xi_f, \{N_{ka}\}_f | \sum_{i < j} V_{ij}^d | \xi_i, \{N_{kd}\}_i \rangle \right|^2. \quad (31)$$

The quotation marks indicate that the energy-conserving function "δ" becomes equal to Dirac's δ function only in the thermodynamical limit. The rate constants $G_{dd \rightarrow \kappa\lambda}(B, T)$ are found by thermal averaging over all possible initial states. As explained in Sec. II B this leads to

$$G_{dd \rightarrow \kappa\lambda}(B, T) = \frac{1}{n^2 V} \sum_{\{N_{k_d}\}_i} \Gamma_{dd \rightarrow \kappa\lambda}(\xi_i, \{N_{k_d}\}_i) \frac{e^{-\beta[E(\xi_i, \{N_{k_d}\}_i) - \mu(\xi_i)N_{sp}(\{N_{k_d}\}_i)]}}{Z_{gr}(\xi_i)}. \quad (32)$$

Note the different roles played by ξ_i and ξ_f : although we restrict ourselves to one ξ_i , ξ_f can still have various values, depending on the number of condensate particles participating in the collision.

We proceed to calculate $G_{dd \rightarrow \kappa\lambda}$ for all five possible processes that are allowed by the selection rules [cf. Eq. (29)] of the electron-electron dipole interaction: $dd \rightarrow aa$, $dd \rightarrow ac$, $dd \rightarrow cc$, $dd \rightarrow ad$, and $dd \rightarrow cd$. Denoting the magnetic-field-dependent change of internal energy in the reaction $dd \rightarrow \kappa\lambda$ by $\Delta_{\kappa\lambda}$ we will give in Sec. III A an expansion of $G_{dd \rightarrow \kappa\lambda}$ in terms of $k_B T / \Delta_{\kappa\lambda}$, which for most practical purposes can be considered as a small quantity. However, near the center of the trap the magnetic field strength is of the order of a few gauss, leading to small energy splittings $\Delta_{cd} \simeq \mu_e B$ and $\Delta_{cc} \simeq 2\mu_e B$. With this application in mind it is also interesting to look at small $\Delta_{\kappa\lambda}$ and even at the extreme case $\Delta_{\kappa\lambda} = 0$. To this end we consider in Sec. III B the transitions $dd \rightarrow cc$ and $dd \rightarrow cd$ at zero magnetic field.

A. The case $\Delta_{\kappa\lambda} \gg k_B T$

To evaluate the quantities $\Gamma_{dd \rightarrow \kappa\lambda}$ and $G_{dd \rightarrow \kappa\lambda}$ we will apply in this and Sec. III B the particlelike (Hartree-Fock) approximation to the dispersion relation of the quasiparticles,

$$\epsilon_{k_d} \simeq \epsilon_{k_d}^0 + \frac{n \xi v_{dd}^{id}}{2} = \epsilon_{k_d}^0 + k_B T O(na \Lambda^2 \xi), \quad (33)$$

leading to a trivial Bogoliubov transformation: The quasiparticle operators $b_{k_d}^\dagger$ and b_{-k_d} are equal to $a_{k_d}^\dagger$ and a_{-k_d} , respectively. Furthermore, in the nondiagonal matrix element of Eq. (31) we again neglect the fluctuations of the condensate fraction, which amounts to the replacement of a_{0d}^\dagger and a_{0d} by the c number $\sqrt{\xi N}$.

We then find, for a specific process $dd \rightarrow \kappa\lambda$ ($\kappa \neq d$),

$$\begin{aligned} \Gamma_{dd \rightarrow \kappa\lambda}(\xi, \{N_{k_d}\}) = & \frac{2\pi}{\hbar} \left[\frac{\xi^2 N^2}{V^2} \frac{1}{(1 + \delta_{\kappa\lambda})} \sum_{\mathbf{q}} |V_{\kappa\lambda, dd}^d(\mathbf{q})|^2 (N_{-q_d} \delta_{\lambda d} + 1) \delta''(\Delta_{\kappa\lambda}^{(2)} E) \right. \\ & + \frac{\xi N}{V^2} \frac{1}{(1 + \delta_{\kappa\lambda})} \sum_{\mathbf{q}} |V_{\kappa\lambda, dd}^d(\mathbf{q}) + V_{\kappa\lambda, dd}^d(\mathbf{q} + \mathbf{k})|^2 (N_{-q_d} \delta_{\lambda d} + 1) N_{k_d} \delta''(\Delta_{\kappa\lambda}^{(1)} E) \\ & \left. + \frac{1}{V^2} \frac{1}{2(1 + \delta_{\kappa\lambda})} \sum_{\mathbf{k}, \mathbf{k}' \neq 0} |V_{\kappa\lambda, dd}^d(\mathbf{q}) + V_{\kappa\lambda, dd}^d(\mathbf{q} + \mathbf{k} - \mathbf{k}')|^2 \right. \\ & \left. \times (N_{\mathbf{k}' - q_d} \delta_{\lambda d} + 1) N_{k_d} N_{k'_d} \delta''(\Delta_{\kappa\lambda}^{(0)} E) \right], \quad (34) \end{aligned}$$

where the factors $(1 + \delta_{\kappa\lambda})^{-1}$ and $[2(1 + \delta_{\kappa\lambda})]^{-1}$ assure that the incoherent summations over final momenta are effectively over distinguishable states. The three contributions to $\Gamma_{dd \rightarrow \kappa\lambda}$ correspond to a collision between two condensate particles, between one condensate and one noncondensate particle, and between two noncondensate particles. The values of ξ_f involved are equal to $\xi_i - 2/N$, $\xi_i - 1/N$, and ξ_i , respectively. Furthermore, the energy differences are

$$\begin{aligned} \Delta_{\kappa\lambda}^{(2)} E &= \frac{\hbar^2 \mathbf{q}^2}{m_H} - \Delta_{\kappa\lambda} + k_B T O(na \Lambda^2), \\ \Delta_{\kappa\lambda}^{(1)} E &= \frac{\hbar^2 (\mathbf{k} + \mathbf{q})^2}{2m_H} + \frac{\hbar^2 \mathbf{q}^2}{2m_H} - \frac{\hbar^2 \mathbf{k}^2}{2m_H} - \Delta_{\kappa\lambda} + k_B T O(na \Lambda^2), \\ \Delta_{\kappa\lambda}^{(0)} E &= \frac{\hbar^2 (\mathbf{k} + \mathbf{q})^2}{2m_H} + \frac{\hbar^2 (\mathbf{k}' - \mathbf{q})^2}{2m_H} - \frac{\hbar^2 \mathbf{k}^2}{2m_H} - \frac{\hbar^2 \mathbf{k}'^2}{2m_H} - \Delta_{\kappa\lambda} + k_B T O(na \Lambda^2). \end{aligned} \quad (35)$$

To obtain Eqs. (34) and (35) we need the amount of energy required to remove a particle from the condensate, which is equal to

$$E \left[\xi - \frac{1}{N}, \{N_{k_\alpha}\} \right] - E(\xi, \{N_{k_\alpha}\}).$$

Using the particlelike limit of the dispersion relation, this difference is calculated to be

$$-\frac{1}{N} \frac{d}{d\xi} E(\xi, \{N_{k_\alpha}\}) = \frac{n \xi v_{dd}^{id}}{2} = k_B T O(na \Lambda^2 \xi).$$

In addition, scattering processes that create a condensate

particle in the case $\lambda=d$ are omitted, since momentum and energy cannot be simultaneously conserved if $\Delta_{\kappa d} \gg k_B T$.

The rate constants are now found from Eq. (34) replacing ξ and $N_{\kappa d}$ by their thermal averages $\bar{\xi}$ and $\langle N_{\kappa d} \rangle_{gr}$. The latter is given by the Bose distribution

$$\langle N_{\kappa d} \rangle_{gr} = \frac{1}{\bar{\xi}^{-1} e^{\beta \epsilon_{\kappa d}} - 1}. \quad (36)$$

Due to conservation of energy the influence of the anti-blocking factors ($\langle N_{\kappa d} \rangle_{gr} + 1$) appearing in the resulting expression for $G_{dd \rightarrow \kappa d}$ can also be neglected. The energy $\epsilon_{\kappa d}$ of the quasiparticle produced in the process $dd \rightarrow \kappa d$ at low temperatures is of the order of the hyperfine splitting $\Delta_{\kappa d}$, leading to the estimate

$$\langle N_{\kappa d} \rangle_{gr} \simeq \exp(-\beta \Delta_{\kappa d}) \ll 1$$

for the average occupation.

We now calculate the three contributions $G_{dd \rightarrow \kappa \lambda}^{(n)}$ ($n=0,1,2$ denotes the number of condensate particles involved) to the rate constants by taking the thermodynamical limit and neglecting the $k_B T O(na\Lambda^2)$ terms in the energy difference $\Delta_{\kappa \lambda}^{(n)}$. The first line of Eq. (34) is associated with $n=2$ and leads to

$$\begin{aligned} G_{dd \rightarrow \kappa \lambda}^{(2)}(B, T) &= \frac{4\pi(\mu_0 \mu_e^2)^2}{45} \frac{\bar{\xi}^2}{(2\pi)^2 \hbar} \frac{|\langle \kappa \lambda | \Sigma_{2\Delta_{M_F}}^{ee} | dd \rangle|^2}{1 + \delta_{\kappa \lambda}} \\ &\quad \times \int d\mathbf{q} |Y_{2\Delta_{M_F}}^*(\hat{\mathbf{q}})|^2 \delta(\Delta_{\kappa \lambda}^{(2)} E) \\ &= \frac{\bar{\xi}^2}{2} G_{dd \rightarrow \kappa \lambda}^{MB}(B, T=0). \end{aligned} \quad (37)$$

The quantity $G_{dd \rightarrow \kappa \lambda}^{MB}(B, T=0)$ is the $T \rightarrow 0$ limit of the rate constant using a Maxwell-Boltzmann velocity distribution

$$G_{dd \rightarrow \kappa \lambda}^{(1)}(B, T) = \frac{4\pi(\mu_0 \mu_e^2)^2}{45} \frac{\bar{\xi}}{(2\pi)^2 n \hbar} \frac{|\langle \kappa \lambda | \Sigma_{2\Delta_{M_F}}^{ee} | dd \rangle|^2}{1 + \delta_{\kappa \lambda}} \int d\mathbf{k} \int d\mathbf{q} |Y_{2\Delta_{M_F}}^*(\mathbf{q}) + Y_{2\Delta_{M_F}}^*(\mathbf{q} + \mathbf{k})|^2 \langle N_{\kappa d} \rangle_{gr} \delta(\Delta_{\kappa \lambda}^{(1)} E). \quad (39)$$

By changing the integration variables \mathbf{q} and \mathbf{k} to $\mathbf{p} + \mathbf{p}'$ and $-\mathbf{2p}'$, respectively, and using the isotropy of the thermally averaged occupations numbers, the double integral can be written as

$$8 \int dp p^2 \int dp' p'^2 \langle N_{2p, d} \rangle_{gr} \delta \left[\frac{\hbar^2 p'^2}{m_H} - \frac{\hbar^2 p^2}{m_H} - \Delta_{\kappa \lambda} \right] \int d\hat{\mathbf{p}} \int d\hat{\mathbf{p}}' |Y_{2\Delta_{M_F}}^*(\mathbf{p} + \mathbf{p}') + Y_{2\Delta_{M_F}}^*(\mathbf{p} - \mathbf{p}')|^2.$$

In the Appendix we show that the double integral over the directions of \mathbf{p} and \mathbf{p}' equals

$$4 \sum_{l' \text{ even}} |f_{l'l}(p', p)|^2 \int_{p=0}^{\infty} 16\pi \left[1 - \frac{p^2}{p'^2} + O\left(\frac{p^4}{p'^4}\right) \right], \quad (40)$$

where the functions $f_{l'l}(p', p)$ characterized a transition (induced by the dipole interaction) from a two-body state with relative momentum p and relative angular momentum l to a similar state with p' and l' . Collecting these results we find

$$G_{dd \rightarrow \kappa \lambda}^{(1)}(B, T) = 2\bar{\xi}(1 - \bar{\xi}) G_{dd \rightarrow \kappa \lambda}^{MB}(B, T=0) \left[1 - \frac{9}{8} \frac{g_{5/2}(\bar{\xi})}{g_{3/2}(\bar{\xi})} \frac{k_B T}{\Delta_{\kappa \lambda}} + O\left(\left[\frac{k_B T}{\Delta_{\kappa \lambda}}\right]^2\right) \right]. \quad (41)$$

In principle, the argument of the Bose functions should be $\bar{\xi} \exp(-\beta v_{dd}^{id} \bar{\xi}/2)$ instead of $\bar{\xi}$. However, the relative

contribution for the atoms in the gas and the plane-wave Born approximation (PWBA) to the transition amplitude. It gives an excellent description of the decay of the doubly spin-polarized gas in the temperature regime $T_c \ll T \ll \Delta_{\kappa \lambda}/k_B$ and for magnetic field strengths $B \lesssim 0.1 \text{ T}$.⁸ Explicitly it reads

$$G_{dd \rightarrow \kappa \lambda}^{MB}(B, T=0) = \frac{m_H (\mu_0 \mu_e^2)^2}{90\pi \hbar^3} \left[\frac{m_H \Delta_{\kappa \lambda}}{\hbar^2} \right]^{1/2} \times |\langle \kappa \lambda | \Sigma_{2\Delta_{M_F}}^{ee} | dd \rangle|^2, \quad (38)$$

introducing the symmetrized and normalized spin states $|\{\alpha\beta\}\rangle$ of Ref. 8. Actually, Eq. (38) is a direct generalization of the expressions found by van den Eijnde¹⁹ and Ruckenstein,²⁰ who considered the case of $bb \rightarrow ab$ relaxation, relevant to the earlier experiments with $H \downarrow \uparrow$.

At zero temperature all particles are in the condensate ($\bar{\xi}=1$) and only collisions with $n=2$ are possible. Hence from Eq. (37) we can already conclude that in this limit all decay rates decrease by a factor of 2. This is easily explained by the following symmetry argument. In the classical regime all occupation numbers are small compared to 1, so that it is highly improbable to find two atoms in the same state $|\kappa d\rangle$. Therefore, if two atoms (i and j) collide, they are in the normalized symmetric state

$$(|\kappa d\rangle_i \otimes |\kappa d\rangle_j + |\kappa d\rangle_j \otimes |\kappa d\rangle_i) / \sqrt{2}.$$

In the $T \rightarrow 0$ limit \mathbf{k} and \mathbf{k}' become zero and this state goes to $\sqrt{2}|0d\rangle_i \otimes |0d\rangle_j$, which results in a transition probability that is a factor of $(\sqrt{2})^2=2$ too large because the correct normalized state would be $|0d\rangle_i \otimes |0d\rangle_j$.

For nonzero temperatures we need to consider also $G^{(1)}$ and $G^{(0)}$. For $G_{dd \rightarrow \kappa \lambda}^{(1)}$ we obtain

difference of the two is of the order $na\Lambda^2\bar{\xi}$ and negligible.

The evaluation of $G_{dd\rightarrow\kappa\lambda}^{(0)}$ proceeds similarly. After taking the thermodynamical limit we transform from initial momenta \mathbf{k} and \mathbf{k}' to center-of-mass and relative momenta \mathbf{P} and \mathbf{p} and write the transferred momentum \mathbf{q} as the difference $\mathbf{p}' - \mathbf{p}$ between final and initial relative momenta. This gives

$$G_{dd\rightarrow\kappa\lambda}^{(0)}(B, T) = \frac{4\pi(\mu_0\mu_c^2)^2}{45} \frac{1}{(2\pi)^8 n^2 \hbar} \frac{|\langle \kappa\lambda | \Sigma_{2\Delta M_F}^{\epsilon\epsilon} | dd \rangle|^2}{2(1 + \delta_{\kappa\lambda})} \times \int d\mathbf{p} \int d\mathbf{p}' \left[\int d\mathbf{P} \langle N_{\mathbf{P}/2+\mathbf{p}, d} \rangle_{gr} \langle N_{\mathbf{P}/2-\mathbf{p}, d} \rangle_{gr} \right] \delta \left[\frac{\hbar^2 \mathbf{p}'^2}{m_H} - \frac{\hbar^2 \mathbf{p}^2}{m_H} - \Delta_{\kappa\lambda} \right] \times |Y_{2\Delta M_F}^*(\mathbf{p} + \mathbf{p}') + Y_{2\Delta M_F}^*(\mathbf{p} - \mathbf{p}')|^2. \tag{42}$$

We note that the function in the first pair of large parentheses, which is up to the factor $[n(2\pi)^3]^{-1}$ equal to the distribution function for the relative momentum \mathbf{p} , is independent of the direction of \mathbf{p} . Therefore it is possible to first carry out the integrations over \mathbf{p}' and the direction of \mathbf{p} and subsequently use the expansion (40). Finally, reintroducing \mathbf{k} and \mathbf{k}' as integration variables it is possible to express our result in terms of, in particular, the average single-particle kinetic energy. This leads to

$$G_{dd\rightarrow\kappa\lambda}^{(0)}(B, T) = (1 - \bar{\xi})^2 G_{dd\rightarrow\kappa\lambda}^{MB}(B, T=0) \left[1 - \frac{9}{4} \frac{g_{5/2}(\bar{\xi})}{g_{3/2}(\bar{\xi})} \frac{k_B T}{\Delta_{\kappa\lambda}} + O \left[\left(\frac{k_B T}{\Delta_{\kappa\lambda}} \right)^2 \right] \right], \tag{43}$$

if we omit $O(na\Lambda^2\bar{\xi})$ terms in the argument of the Bose functions.

For temperatures above T_c the condensate is absent and only $G_{dd\rightarrow\kappa\lambda}^{(0)}$ survives. In particular, in the classical regime $T_c \ll T \ll \Delta_{\kappa\lambda}/k_B$ the fugacity becomes very small ($\bar{\xi} \ll 1$) and we find for the rate constant

$$G_{dd\rightarrow\kappa\lambda}(B, T) \equiv G_{dd\rightarrow\kappa\lambda}^{MB}(B, T) = G_{dd\rightarrow\kappa\lambda}^{MB}(B, T=0) \left[1 - \frac{9}{4} \frac{k_B T}{\Delta_{\kappa\lambda}} + O \left[\left(\frac{k_B T}{\Delta_{\kappa\lambda}} \right)^2 \right] \right], \tag{44}$$

in complete agreement with the PWBA calculations of van den Eijnde¹⁹ and Ruckenstein.²⁰ This is not surprising, since for $\bar{\xi}=0$ the quasiparticle Hamiltonian (14) reduces to an independent particle Hamiltonian. The deviation of Eq. (43) from Eq. (44) is due to the fact that the average kinetic energy of an ideal gas of bosons is not equal to $\frac{3}{2}k_B T$, as in the case of distinguishable particles,

but equal to

$$\frac{3}{2}k_B T [g_{5/2}(\bar{\xi})/g_{3/2}(\bar{\xi})].$$

In the present practical realizations of a magnetic trap the largest part of the trapping region has such high magnetic field values that $\Delta_{\kappa\lambda} \gg k_B T$ for temperatures around T_c . In these circumstances even the linear terms

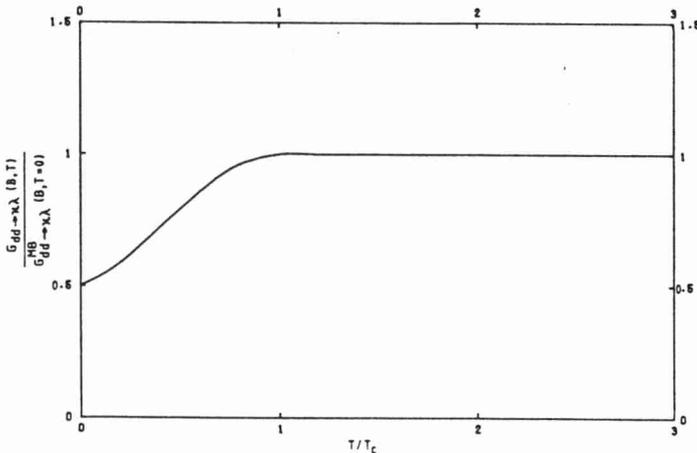


FIG. 3. Temperature dependence of relaxation rates $G_{dd\rightarrow\kappa\lambda}$ at large magnetic fields.

in the parameter $k_B T / \Delta_{\kappa\lambda}$ can be neglected and the rate constant reduces to

$$G_{dd \rightarrow \kappa\lambda}(B, T) = \frac{1}{2}(2 - \bar{\xi}^2) G_{dd \rightarrow \kappa\lambda}^{\text{MB}}(B, T=0). \quad (45)$$

The temperature dependence of the decay rates is then fully described by the function $(2 - \bar{\xi}^2)/2$, which is shown in Fig. 3. Note that here deviations due to the Bose character of the velocity distribution of the hydrogen atoms only appear at temperatures below T_c and are maximal when $T=0$. As mentioned above, at zero temperature the rate of decay is smaller by a factor of 2. From the discussion following Eq. (38) it is clear that for an N -body process the transition probability is reduced by $1/N!$. The corresponding factor of 6 reduction in the case of three-body recombination (the dominant decay channel in $H \downarrow \uparrow$) was first noticed by Kagan *et al.*¹⁰ Applying their method to the case of two-body relaxation processes, we find that the dominant temperature dependence is given by the correlator K , which in terms of field operators $\Psi(\mathbf{r})$ is equal to

$$K = \frac{1}{2n^2} \langle \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \Psi(\mathbf{r}) \rangle, \quad (46)$$

$$G_{dd \rightarrow \kappa\lambda}(B, T) = G_{dd \rightarrow \kappa\lambda}^{\text{MB}}(B, T=0) \left[\frac{1}{2} \bar{\xi}^2 + 2 \bar{\xi} (1 - \bar{\xi}) \left[1 - \frac{9}{8} \frac{g_{5/2}(\bar{\xi})}{g_{3/2}(\bar{\xi})} \frac{k_B T}{\Delta_{\kappa\lambda}} + \dots \right] + (1 - \bar{\xi})^2 \left[1 - \frac{9}{4} \frac{g_{5/2}(\bar{\xi})}{g_{3/2}(\bar{\xi})} \frac{k_B T}{\Delta_{\kappa\lambda}} + \dots \right] \right] \quad (47)$$

to obtain accurate results. For a realistic situation with a magnetic field of 5 G and a density of 10^{14} cm^{-3} ($T_c \approx 34 \mu\text{K}$) we give in Fig. 4 the rates $G_{dd \rightarrow cc}(B, T)$ and $G_{dd \rightarrow cc}^{\text{MB}}(B, T)$ as a function of T/T_c . Similar results are

valid for the $dd \rightarrow cd$ process. In these cases deviations due to the proper use of Bose statistics already appear for temperatures above T_c . Although the effect is small and the decay rates for the processes $dd \rightarrow aa$, $dd \rightarrow ac$, and

$$\Psi(\mathbf{r}) = (\bar{\xi}n)^{1/2} + \Psi'(\mathbf{r}),$$

and using the identity

$$(1 - \bar{\xi})n = \langle \Psi^\dagger(\mathbf{r}) \Psi'(\mathbf{r}) \rangle,$$

the correlator is calculated to be $\frac{1}{2}(2 - \bar{\xi}^2)$. This agrees with our results to lowest order in $k_B T / \Delta_{\kappa\lambda}$. One does not expect to find agreement in higher orders, because Kagan *et al.* assume the classical (Maxwell-Boltzmann) results to be temperature independent. Note also that, contrary to Kagan *et al.*'s three-body rate, our rates have a continuous first derivative at $T = T_c$. The discontinuity appears in our case in the second derivative.

In the center of the trap we have such small magnetic fields that the hyperfine splitting between the $|d\rangle$ and $|c\rangle$ states becomes comparable to the thermal energy. Then the linear terms in $k_B T / \Delta_{\kappa\lambda}$ must be retained and we need

valid for the $dd \rightarrow cd$ process. In these cases deviations due to the proper use of Bose statistics already appear for temperatures above T_c . Although the effect is small and the decay rates for the processes $dd \rightarrow aa$, $dd \rightarrow ac$, and

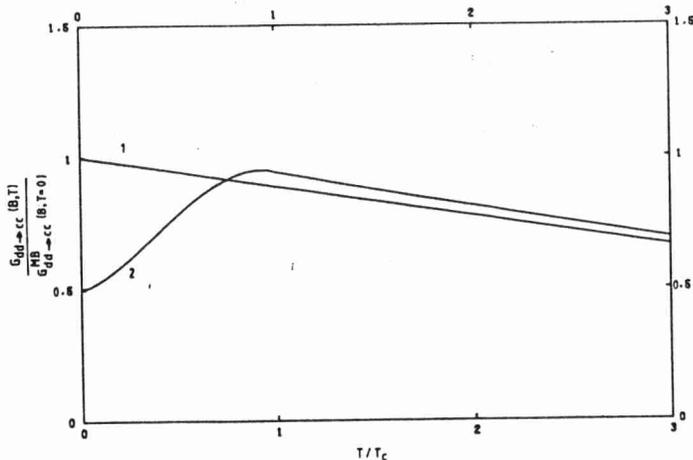


FIG. 4. Temperature dependence of relaxation rate $G_{dd \rightarrow cc}$ at a magnetic field of 5 G and a density of 10^{-14} cm^{-3} . Curve 1, without Bose-Einstein condensation and using a Maxwell-Boltzmann velocity distribution. Curve 2, with Bose-Einstein condensation.

$dd \rightarrow ad$ are roughly an order of magnitude larger than those for $dd \rightarrow cc$ and $dd \rightarrow cd$, this precursor effect may prove useful to study the approach to the Bose-Einstein transition.

Finally, in connection with Ref. 20 we would like to point out that Ruckenstein considers $bb \rightarrow ab$ relaxation also at temperatures below T_c . However, he considers the somewhat unrealistic situation of a gas of a and b atoms ($H \downarrow$) in thermal equilibrium neglecting the important mechanism of preferential recombination leading to the formation of the doubly spin-polarized gas. In this case the Bose condensation takes place in the one-atom ground state, i.e., the state $|0a\rangle$. Therefore Ruckenstein finds that $G_{bb \rightarrow ab}$ consists of two contributions with a different temperature dependence. One is proportional to $\bar{\xi}$ and the other to $1 - \bar{\xi}$. It is in this respect important to point out that, as can easily be seen from our physical picture of the decrease of $G_{dd \rightarrow \kappa\lambda}$ by a factor of 2, to lowest order in $k_B T / \Delta_{ab}$ the Bose character of the hydrogen atoms does not affect the decay of the gas, since we have

$$G_{bb \rightarrow ab}(B, T) = G_{bb \rightarrow ab}^{MB}(B, T=0) [\bar{\xi} + (1 - \bar{\xi})] = G_{bb \rightarrow ab}^{MB}(B, T=0).$$

If we do take preferential recombination into account and

$$G_{dd \rightarrow cc}^{(1)}(B=0, T) = \frac{4\pi(\mu_0 \mu_e^2)^2 m_H}{45 \cdot 8\pi^2 \hbar^3} \left[\frac{m_H k_B T}{2\pi \hbar^2} \right]^{1/2} |\langle cc | \Sigma_{2,-2}^{ee} | dd \rangle|^2 \frac{g_2(\bar{\xi})}{g_{3/2}(\bar{\xi})} \bar{\xi}(1 - \bar{\xi}) \\ \equiv \sqrt{2} \bar{\xi}(1 - \bar{\xi}) G_{dd \rightarrow cc}^{MB}(B=0, T) \frac{g_2(\bar{\xi})}{g_{3/2}(\bar{\xi})}. \tag{48}$$

Similarly, after a straightforward but elaborate calculation $G_{dd \rightarrow cc}^{(0)}$ becomes

$$G_{dd \rightarrow cc}^{(0)}(B=0, T) = \frac{4\pi(\mu_0 \mu_e^2)^2 m_H}{45 \cdot 8(2\pi)^3 \hbar^3} |\langle cc | \Sigma_{2,-2}^{ee} | dd \rangle|^2 \int d\mathbf{k} \int d\mathbf{k}' |\mathbf{k} - \mathbf{k}'| \langle N_{\mathbf{k}d} \rangle_{gr} \langle N_{\mathbf{k}'d} \rangle_{gr} \\ = 2\sqrt{2}(1 - \bar{\xi})^2 G_{dd \rightarrow cc}^{MB}(B=0, T) \frac{h_{5/2,1}(\bar{\xi}) + \frac{1}{2} h_{3/2,2}(\bar{\xi})}{g_{3/2}(\bar{\xi})}, \tag{49}$$

where we introduced the functions $h_{n,m}(\xi)$. They are defined by

$$h_{n,m}(\xi) \equiv \sum_{i=2}^{\infty} \frac{1}{i^n} \left[\sum_{j=1}^{i-1} \frac{1}{j^m} \right] \xi^i \\ = \frac{1}{\Gamma(p)} \int_0^{\infty} dy \frac{y^{n-1}}{\xi^{-1} e^y - 1} g_m(\xi e^{-y}) \tag{50}$$

and can easily be calculated numerically. Those occurring in Eq. (49) are shown in Fig. 5. Note for $\xi \rightarrow 0$ the functions $h_{n,m}(\xi)$ behave as $2^{-n} \xi^{2-n}$. Consequently, if $T \gg T_c$ the rate $G_{dd \rightarrow cc}(B=0, T)$ reduces to the classical result $G_{dd \rightarrow cc}^{MB}(B=0, T)$. This feature can also be seen in Fig. 6, in which we give both rate constants.

For the process $dd \rightarrow cd$ at zero magnetic field the evaluation of the decay rates requires elaborate numerical calculations, because the antiblocking factors in Eq. (34) are involved in the integral over \hat{p} and \hat{p}' . In the most difficult case we have a ninefold integral over \mathbf{P} , \mathbf{p} , and \mathbf{p}'

consider a gas of b atoms, then Eq. (47) is applicable and we find a deviation from classical behavior. Unfortunately, the dominant decay mechanism is now three-body recombination both in the bulk and on the liquid-helium surface, which prevents the accurate determination of the relaxation rates near the phase transition.

B. The case $\Delta_{\kappa\lambda} = 0$

Although one avoids zero-field regions experimentally to suppress Majorana spin flips, we consider the process $dd \rightarrow cc$ as an example of what may happen if such regions are present. We can still apply the completely general Eqs. (37), (39), and (42) and neglect the $k_B T O(na\Lambda^2)$ terms in $\Delta_{cc}^{(n)} E$, because the relevant thermal energies are of the order $k_B T$. First of all we conclude that $G_{dd \rightarrow cc}^{(2)} = 0$. For the calculation of $G_{dd \rightarrow cc}^{(1)}$ and $G_{dd \rightarrow cc}^{(0)}$ we again need the integral over the directions of \mathbf{p} and \mathbf{p}' ,

$$\int d\hat{p} \int d\hat{p}' |Y_{2,-2}^*(\mathbf{p} + \mathbf{p}') + Y_{2,-2}^*(\mathbf{p} - \mathbf{p}')|^2,$$

but now with equal magnitudes of the momenta \mathbf{p} and \mathbf{p}' . In the Appendix we find that in this situation the integral is equal to 4π . We are thus able to reduce the double momentum integral in Eq. (39) to Bose functions with the result

which cannot be handled analytically and may be calculated using Monte Carlo techniques. We therefore do not consider it here.

IV. CONCLUSIONS

We modified the ξ -method of Lee and Yang to analyze the decay of doubly spin-polarized atomic hydrogen in a static magnetic trap. We assumed that the translational degrees of freedom of the atoms are in thermal equilibrium and calculated all dipolar relaxation rates $G_{dd \rightarrow \kappa\lambda}$ as a function of temperature and applied magnetic field. Our results are correct to lowest order in the parameters $(na^3)^{1/4}$, $(na\Lambda^2)^{1/2}$, and $(a/n\Lambda^4)^{1/4}$, which is sufficiently accurate for all practically accessible temperatures and densities. Most importantly we find that the decay probability has a discontinuous second derivative with respect to temperature at $T = T_c$ and decreases well below the transition point by a factor of 2. In addition, we show

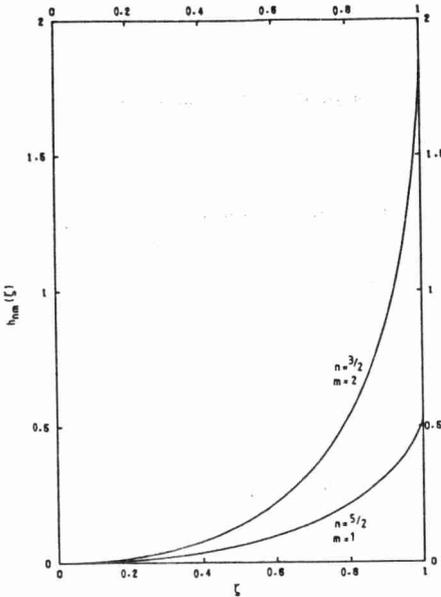


FIG. 5. Functions $h_{n,m}(\zeta)$ for $(n=3/2, m=1)$ and $(n=5/2, m=2)$.

that for sufficiently small magnetic fields also precursor effects occur. All these phenomena may be of importance to studying the approach and realization of the Bose-Einstein transition.

APPENDIX

To calculate the contribution $G_{dd \rightarrow \kappa\lambda}^{(0)}$ and $G_{dd \rightarrow \kappa\lambda}^{(1)}$ to the decay rates $G_{dd \rightarrow \kappa\lambda}$ we have to evaluate the integral

$$\int d\hat{p} \int d\hat{p}' |Y_{2\mu}(\mathbf{p}+\mathbf{p}') + Y_{2\mu}(\mathbf{p}-\mathbf{p}')|^2,$$

with $\mu = -\Delta M_F$. To this end we expand the spherical harmonic $Y_{2\mu}(\mathbf{p}+\mathbf{p}')$ in terms of the functions $\mathcal{Y}_{ll'}^{LM}(\hat{p}, \hat{p}')$, which are formed from separate spherical harmonics by angular momentum coupling:

$$\mathcal{Y}_{ll'}^{LM}(\hat{p}, \hat{p}') = \sum_{mm'} (lm'l'm'|LM) Y_{lm}(\hat{p}) Y_{l'm'}(\hat{p}'). \quad (A1)$$

The desired expansion reads

$$Y_{2\mu}(\mathbf{p}+\mathbf{p}') = \sum_{ll'} f_{ll'}(p', p) \mathcal{Y}_{ll'}^{2\mu}(\hat{p}, \hat{p}'), \quad (A2)$$

with the coefficients $f_{ll'}(p', p)$ obeying

$$f_{ll'}(p', p) = \int d\hat{p} \int d\hat{p}' \mathcal{Y}_{ll'}^{2\mu}(\hat{p}, \hat{p}') Y_{2\mu}(\mathbf{p}+\mathbf{p}'). \quad (A3)$$

Using the convenient notation $\hat{l} = 2l + 1$ and the formula¹³

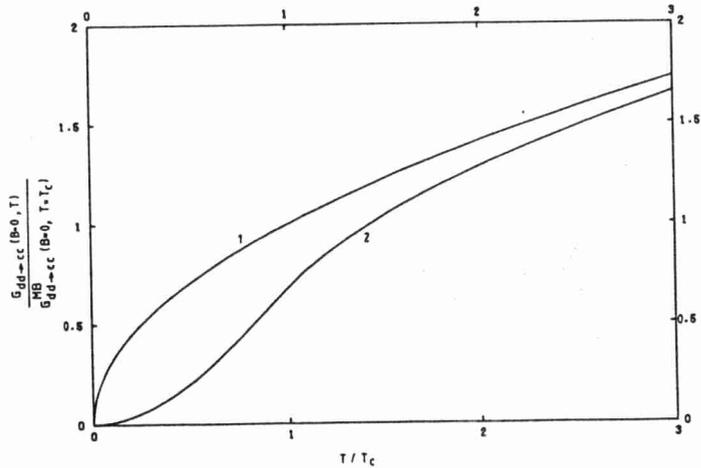


FIG. 6. Temperature dependence of relaxation rate $G_{dd \rightarrow \kappa\kappa}$ at zero magnetic field. Curve 1, without Bose-Einstein condensation and using a Maxwell-Boltzmann velocity distribution. Curve 2, with Bose-Einstein condensation.

$$Y_{lm}(\mathbf{p}+\mathbf{p}') = \sum_{l_1+l_2=l} \frac{p^{l_1} p'^{l_2}}{|\mathbf{p}+\mathbf{p}'|^l} \left[\frac{4\pi\hat{\Pi}}{\hat{l}_1\hat{l}_2!} \right]^{1/2} \mathcal{Y}_{l_1 l_2}^m(\hat{\mathbf{p}}, \hat{\mathbf{p}}'), \quad (\text{A4})$$

we are able to carry out the integrations over the directions of \mathbf{p} and \mathbf{p}' analytically if we expand also $|\mathbf{p}+\mathbf{p}'|^{-2}$ in terms of spherical harmonics:

$$\frac{1}{|\mathbf{p}+\mathbf{p}'|^2} \frac{2\pi}{pp'} \sum_{l''} (-1)^{l''} Q_{l''}(z) \sum_{m''} Y_{l'' m''}^*(\hat{\mathbf{p}}) Y_{l'' m''}(\hat{\mathbf{p}}'), \quad (\text{A5})$$

where $Q_{l''}(z)$ are Legendre functions of the second kind²¹ and $z = (p^2 + p'^2)/2pp'$. After some Racah algebra we finally obtain

$$f_{l'l}(p', p) = 2(30\pi\hat{\Pi}')^{1/2} \sum_{l''} \hat{l}'' Q_{l''}(z) \sum_{l_1+l_2=2} \frac{p^{l_1-1} p'^{l_2-1}}{\sqrt{(2l_1)!(2l_2)!}} \begin{Bmatrix} l & l_1 & l'' \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l'' & l_2 & l' \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l & l' & 2 \\ l_2 & l_1 & l'' \end{Bmatrix}, \quad (\text{A6})$$

and

$$\int d\hat{\mathbf{p}} \int d\hat{\mathbf{p}}' |Y_{2\mu}(\mathbf{p}+\mathbf{p}') + Y_{2\mu}(\mathbf{p}-\mathbf{p}')|^2 = 4 \sum_{l'' \text{ even}} |f_{l'l}(p', p)|^2, \quad (\text{A7})$$

making use of the selection rules of the Wigner $3-j$ and $6-j$ symbols in Eq. (A6).

The special case $p=p'$, needed when $\Delta_{\lambda\lambda}=0$, has to be considered separately because the Legendre functions $Q_{l''}(z)$ diverge logarithmically if $z=1$. However, if we split off the logarithmic part and write $Q_{l''}(z)$ as²¹

$$Q_{l''}(z) = \frac{1}{2} P_{l''}(z) \ln \left[\frac{z+1}{z-1} \right] - W_{l''-1}(z), \quad (\text{A8})$$

with $P_{l''}(z)$ a Legendre function of the first kind and

$$W_{l''-1}(z) = \frac{1}{2} \int_{-1}^1 dx \frac{P_{l''}(z) - P_{l''}(x)}{z-x},$$

we find that the divergent parts cancel. Equation (A6) thus reduces to

$$f_{l'l}(p, p) = -2(30\pi\hat{\Pi}')^{1/2} \sum_{l''} \hat{l}'' W_{l''-1}(1) \sum_{l_1+l_2=2} \frac{1}{\sqrt{(2l_1)!(2l_2)!}} \begin{Bmatrix} l & l_1 & l'' \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l'' & l_2 & l' \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l & l' & 2 \\ l_2 & l_1 & l'' \end{Bmatrix}. \quad (\text{A9})$$

Substituting $W_{l''-1}(1) = \sum_{i=1}^{l''} i^{-1}$ we find that

$$\int d\hat{\mathbf{p}} \int d\hat{\mathbf{p}}' |Y_{2\mu}(\mathbf{p}+\mathbf{p}') + Y_{2\mu}(\mathbf{p}-\mathbf{p}')|^2 = 4 \sum_{l'' \text{ even}} [|f_{l-2,l}(p, p)|^2 + |f_{l,l}(p, p)|^2 + |f_{l+2,l}(p, p)|^2] = 4\pi, \quad (\text{A10})$$

if $p=p'$.

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Nonsingular integral equation for two-body scattering and applications in two and three dimensions

H. T. C. Stoof, L. P. H. de Goeij, W. M. H. M. Rovers, P. S. M. Kop Jansen, and B. J. Verhaar
Department of Physics, Eindhoven University of Technology, NL-5600 MB Eindhoven, The Netherlands
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We introduce a new nonsingular scattering integral equation, which is suitable for the investigation of the total (also off-shell) transition matrix in arbitrary dimension $n \geq 2$. In particular, the low-energy properties are derived and lead, in connection with spin-polarized atomic hydrogen H I, to the low-temperature behavior of two- and three-body surface processes. In addition, for all dimensions the method leads in a natural way to a separable approximation to the T matrix for three energies, with the possibility of formulating a procedure for optimizing this approximation. To show the practicability of the equation we also present numerical results for both $n = 2$ and $n = 3$.

I. INTRODUCTION

In the last decade the preparation and study of two-dimensional systems has attracted a great deal of attention. Surface physics with its development of new sensitive detection techniques such as the scanning tunneling microscope, two-dimensional electron gases exhibiting the integral and fractional quantum Hall effect, and high- T_c superconductors, in which the layer structure of the lattice may play an important role in the pairing mechanism, are just a few examples of the increasing interest in this field of physics.

Another experimentally accessible two-dimensional system is low-temperature spin-polarized atomic hydrogen (H I) that is adsorbed at a surface of liquid helium.¹ The two-dimensional gas plays a vital role in connection with experiments aiming at Bose-Einstein condensation: At temperatures below about 0.3 K the density of the adsorbed gas is so high that the stability of the gas sample as a whole is mainly determined by two-dimensional relaxation and recombination processes. Indeed, the three-body recombination on the helium surface is the main cause of the inability of the conventional compression experiments to achieve the Bose-Einstein transition in the H I gas.² To circumvent this dominant decay process, it is important to understand the physical mechanism through which the recombination proceeds and hence to be able to predict the magnetic field and low-temperature behavior of the surface recombination rate constant L_s . However, formulating a Faddeev formalism for this three-body problem in two dimensions, as was done in the volume case,³ leads to substantial problems caused by the logarithmic energy dependence of the two-dimensional two-body T (transition) operator.

As a first step in solving the above-mentioned problems and arriving at a three-body effective-range theory, we introduce in Sec. II a new method to study the complete T matrix and in particular its energy dependence. The most important results, needed for subsequent applications, are given in Eqs. (4) and (7). We formulate the

method in arbitrary dimension and apply it to two and three dimensions. Sections III and IV are devoted to two-dimensional scattering and we here discuss the complete agreement of our method with the effective-range theory formulated previously⁴ and derive some preliminary results on the low-temperature behavior of the three-body decay rate L_s . After that we turn in Sec. V to the three-dimensional case and derive a separable approximation to the T matrix for both positive and negative energies. This approximation may be of some use in connection with the solution of Faddeev or Alt-Grassberger-Sandhas (AGS) equations⁵ in, for example, nuclear physics, where a one-term separable expansion is already highly accurate.

II. τ MATRIX

The T matrix in dimension $n \geq 2$ and for a (integer-valued) partial wave l obeys a Lippmann-Schwinger equation⁵ that in the momentum representation takes the form

$$T_l(p, p', E) = V_l(p, p') + \int_0^\infty dp'' (p'')^{n-1} V_l(p, p'') \times \frac{1}{E + (p'')^2/2\mu} \times T_l(p'', p', E). \quad (1)$$

Here μ is the reduced mass of the two colliding particles, E is the total energy available, and the angular momentum associated with the partial wave l is $\sqrt{l(l+n-2)}\hbar$. We assume the interaction to be local and rotationally invariant, in which case all partial waves are decoupled from one another and the (real) momentum representation of the potential $V(r)$ turns out to be

$$V_l(p, p') = \frac{4}{\Gamma^2(\frac{1}{2}n)(2\hbar)^n} \int_0^\infty dr r^{n-1} j_{l,n}(pr/\hbar) V(r) \times j_{l,n}(p'r/\hbar). \quad (2)$$

The functions $j_{l,n}(z)$ play an important role in a generalization of quantum-mechanical scattering theory to arbitrary dimension. They are the solution of a radial Schrödinger equation with the centrifugal barrier

$$\frac{\hbar^2}{2\mu r^2} [(l + \frac{1}{2}n - 1)^2 - \frac{1}{4}]$$

and are related to Bessel functions of the first kind $J_\nu(z)$ by

$$j_{l,n}(z) \equiv \Gamma(\frac{1}{2}n) \left[\frac{2}{z} \right]^{(1/2)n-1} J_{l+(1/2)n-1}(z). \quad (3)$$

The coefficient is chosen such that $j_{0,n}(0)=1$. Furthermore, with this choice these functions reduce in three dimensions to the conventional⁵ spherical Bessel functions $j_l(z)$. For general n relations (1) and (2) imply the symmetry of $V_l(p,p')$ and $T_l(p,p',E)$ in the momentum variables. For convenience we use from now on units such that $\hbar=2\mu=1$ and in addition suppress the subscript l .

In the case of positive energies $E \geq 0$ the notation $E^\pm = E + i0$ used in Eq. (1) specifies the usual integration contour around the singularity associated with the energy denominator. However, this singularity can be avoided by introducing a real and symmetrical τ^Λ matrix by the equation

$$\tau^\Lambda(p,p',E) = V(p,p') + \int_0^\infty dp'' \frac{(p'')^{n-1}}{E - (p'')^2} [V(p,p'')\tau^\Lambda(p'',p',E) - \Theta(\Lambda - p'')V(p,k)\tau^\Lambda(k,p',E)]. \quad (4)$$

We denote the on-shell momentum by $k = \sqrt{E}$ and the Heaviside unit-step function by $\Theta(x)$. Note that at $p''=k$, where the denominator vanishes, the quantity in square brackets also vanishes. Moreover, the cutoff parameter $\Lambda > k$ is needed to obtain a convergent integral and will turn out to have an additional advantage in Sec. V for the purpose of optimizing a separable approximation. The relation between the T and τ^Λ matrices is easily found by subtracting and adding

$$V(p,k)T(k,p',E)I_\Lambda(E) \equiv V(p,k)T(k,p',E) \int_0^\Lambda dp'' \frac{(p'')^{n-1}}{E^\pm - (p'')^2} \quad (5)$$

to the right-hand side of the Lippmann-Schwinger equation (1), which leads to

$$T(p,p',E) = V(p,p') + V(p,k)I_\Lambda(E)T(k,p',E) + \int_0^\infty dp'' \frac{(p'')^{n-1}}{E - (p'')^2} [V(p,p'')T(p'',p',E) - \Theta(\Lambda - p'')V(p,k)T(k,p',E)].$$

This equation for the T matrix is identical to that satisfied by

$$\tau^\Lambda(p,p',E) + \tau^\Lambda(p,k,E)I_\Lambda(E)T(k,p',E),$$

which can be obtained by using Eq. (4) once with p' replaced by k and once with p' itself. We thus find the relation

$$T(p,p',E) = \tau^\Lambda(p,p',E) + \tau^\Lambda(p,k,E)I_\Lambda(E)T(k,p',E). \quad (6)$$

From the right-hand side we can eliminate $T(k,p',E)$ by applying the same equation for the special choice $p=k$. The result of the manipulations is

$$\tau^\Lambda(p,p',E) = V(p,p') + V(p,k)\tau^\Lambda(k,p',E)[I_\Lambda(E) - I_\Lambda(E)] + \int_0^\infty dp'' \frac{(p'')^{n-1}}{E - (p'')^2} [V(p,p'')\tau^\Lambda(p'',p',E) - \Theta(\Lambda - p'')V(p,k)\tau^\Lambda(k,p',E)], \quad (8)$$

and, similarly to the derivation of Eq. (6), we obtain a relation between the τ matrices with different cutoffs

$$\tau^\Lambda(p,p',E) = \tau^\Lambda(p,p',E) + \tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E) \times [I_\Lambda(E) - I_\Lambda(E)]. \quad (9)$$

This result implies the Λ independence of the expressions

$$T(p,p',E) = \tau^\Lambda(p,p',E) - \frac{\tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E)}{\tau^\Lambda(k,k,E)} + \frac{\tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E)}{[\tau^\Lambda(k,k,E)]^2} \times \frac{1}{[1/\tau^\Lambda(k,k,E)] - I_\Lambda(E)}. \quad (7)$$

Note that the T matrix is complex only via the function $I_\Lambda(E)$.

To see that the right-hand side of Eq. (7) is indeed independent of the cutoff parameter Λ , we rewrite the defining equation for $\tau^\Lambda(p,p',E)$ as

$$\tau^\Lambda(p,p',E) - \tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E)/\tau^\Lambda(k,k,E), \\ \tau^\Lambda(p,k,E)/\tau^\Lambda(k,k,E), \\ [1/\tau^\Lambda(k,k,E)] - I_\Lambda(E).$$

Hence we have also proven the Λ independence of Eq. (7).

In connection with effective-range theory it is of interest to note that we expect $\tau_l^A(p, p', E)$ to be well behaved as a function of its arguments and to possess an expansion in p, p' , and E close to $p = p' = E = 0$, with only even (odd) powers of p and p' , if l is even (odd). We are led to this because the integral equation for the τ matrix is nonsingular and the interaction $V_l(p, p')$ has a similar Taylor expansion around $p = p' = 0$. For a rigorous proof of this conjecture in the most important case of two dimensions we refer to the Appendix, but in addition our numerical results presented in Sec. III confirm the expectations mentioned. Together with Eq. (7) this property indicates that the singular energy dependence of the T matrix in even dimensions is given by the function $I_\Lambda(E)$, which can be calculated analytically. In two dimensions this leads to a logarithmic behavior of various kinds of scattering quantities, such as the phase shift and the wave function itself.

Finally, we note that the connection (7) between the T and τ matrices reduces to the single expression

$$T(k, k, E) = \frac{1}{[1/\tau^\Lambda(k, k, E)] - I_\Lambda(E)} \quad (10)$$

$$I_\Lambda(E) = -\frac{\pi i k^{n-2}}{2} - \frac{\Lambda^{n-2}}{n-2} - k^2 \frac{\Lambda^{n-4}}{n-4} + \cdots + \cdots - \begin{cases} \frac{k^{n-2}}{2} \ln \left[\frac{\Lambda - k}{\Lambda + k} \right], & n = \text{odd} \\ \frac{k^{n-2}}{2} \ln \left[\frac{\Lambda^2 - k^2}{k^2} \right], & n = \text{even} \end{cases} \quad (12)$$

where the last term included before the curly bracket is $-k^{n-3}\Lambda$ ($n = \text{odd}$) or $-k^{n-4}\Lambda^2$ ($n = \text{even}$). For odd dimensions this yields an analytical behavior near $k = 0$, with

$$\ln \left[\frac{\Lambda - k}{\Lambda + k} \right] = -2 \frac{k}{\Lambda} - \frac{2}{3} \frac{k^3}{\Lambda^3} + \cdots,$$

while for even dimensions a logarithmic dependence results,

$$\ln \left[\frac{\Lambda^2 - k^2}{k^2} \right] = -2 \ln \left[\frac{k}{\Lambda} \right] - \frac{k^2}{\Lambda^2} - \frac{1}{2} \frac{k^4}{\Lambda^4} + \cdots.$$

Restricting ourselves to the lowest partial wave, we also expand $1/\tau^\Lambda(k, k, E)$ in k ,

$$1/\tau^\Lambda(k, k, E) = a_0(\Lambda) + a_2(\Lambda)k^2 + a_4(\Lambda)k^4 + \cdots.$$

Equation (10) then leads to

$$1/T(k, k, E) = \frac{\pi i k^{n-2}}{2} + c_0 + c_2 k^2 + \cdots + \cdots + \begin{cases} c_{n-1} k^{n-1} + \cdots, & n = \text{odd} \\ k^{n-2} \ln(c_{n-1} k) + c_n k^n + \cdots, & n = \text{even} \end{cases} \quad (13)$$

where the last term before the curly bracket is $c_{n-1} k^{n-3}$ ($n = \text{odd}$) or $c_{n-4} k^{n-4}$ ($n = \text{even}$). This agrees completely with the k dependence of $\cot \delta(k)$ found in Refs. 4 and 6. For $n = 2$, in particular, Eq. (13) may be cast into the form

$$1/T(k, k, E) = \frac{\pi i}{2} - \gamma - \ln(ka/2) - \frac{1}{4} r_e^2 k^2 + \cdots, \quad (14)$$

with a the scattering length, r_e the effective range, and $\gamma = 0.577215665 \dots$ Euler's constant. The values of a

for the on-shell T matrix. Comparing with the more familiar expression for $T(k, k, E)$ in terms of the phase shift for n -dimensional scattering, i.e.,

$$T(k, k, E) = \frac{1}{\frac{\pi i k^{n-1}}{2} - \frac{\pi k^{n-2}}{2} \cot \delta(k)}, \quad (11)$$

following from the relation

$$S(k, k, E) = 1 - \pi i k^{n-2} T(k, k, E)$$

between the S and T matrix elements, we are able to relate $\cot \delta(k)$ to the smoothly behaving τ matrix and the simple function $I_\Lambda(E)$. In Sec. III we will study this relation for two-dimensional scattering to derive the effective-range formula of Ref. 4.

III. LOW-ENERGY SCATTERING: ON-SHELL T MATRIX

We now apply the formalism discussed in Sec. II to low-energy scattering. To this end we calculate the function $I_\Lambda(E)$ to be

and r_e can be calculated from the on-shell τ matrix via the equations

$$\ln(ka/2) = -\gamma - a_0(\Lambda) + \ln(k/\Lambda), \quad (15)$$

$$r_e^2 = -4a_2(\Lambda) + 2/\Lambda^2.$$

The numerical results to be presented here and in the following for $n = 2$ are all associated with hydrogen b atoms (having both electron and proton spins down with respect to an external magnetic field) adsorbed on a

superfluid helium surface, in which case the $2\frac{1}{2}$ -dimensional model is commonly used to find the interaction potential of the H atoms.⁷ This potential is shown in Fig. 1 and is calculated by assuming a Mantz-Edwards⁸ interaction potential between the hydrogen atoms and the helium film. We find $a = 2.4a_0$ and $r_e = 13a_0$, in agree-

ment with the values found by integrating the Schrödinger equation and examining⁹ the phase shifts $\delta(k)$. We conclude that the τ method leads to a low-energy dependence of the on-shell T matrix that is in accordance with effective-range theory and can also be used to find accurate results for the expansion parameters.

Also for all other dimensions Eq. (13) may be rewritten in the standard form of the low-energy expansion introduced in Ref. 4. It is of interest to recall that the expansion parameters occurring in this elegant standard form all have the dimension of length; each of them is defined as the radius of an equivalent hard sphere giving rise to this same specific term in the expansion. Adhikari *et al.* point out in a recent publication¹⁰ that such a definition has the disadvantage in the special case of dimension $n = 2$ that a varies between 0 and $+\infty$ when the potential is changed. This contrasts with $n = 3$ where a is known to vary between $-\infty$ and $+\infty$, its sign reflecting the repulsiveness or attractiveness of the potential. The latter connection thus being lost for $n = 2$, Adhikari *et al.* introduce an alternative scattering length parameter a_{AGL} related to a by $a_{AGL} = -\ln(a/R_c)$, where R_c is the "range" of the potential. Apart from the vagueness implied by the arbitrariness in the choice of R_c , especially for interactions decaying slowly with r , it is of interest to note that the positive definiteness of a for $n = 2$ is not as difficult to understand from the physical point of view as Ref. 10 suggests; $n = 2$ is the only integer dimension for which the lowest partial wave $l = 0$ has a negative centrifugal "barrier" extending over a long range.

Also the sign of the phase shift is an aspect in which $n = 2$ differs. For any weak potential, whether predominantly attractive or repulsive, δ is always negative. Further smooth changes of the potential to arbitrary strength cause δ to change continuously, taking negative values only.

Another point of view illustrating the fundamental difference between two- and three-dimensional concepts of scattering length is the following. In varying the depth of a potential well $V(r)$ for $n = 2$ a bound level enters the well precisely at the same potential depth where the phase shift vanishes. In three dimensions this happens at different well depths. This difference is naturally reflected in the different behavior of the corresponding quantity a ; the two a values 0 and $-\infty$ for $n = 3$ merge into a single value 0 when the dimension changes to 2. The quantity a_{AGL} , however, goes through zero for a well depth without a clear-cut physical significance.

IV. LOW-ENERGY SCATTERING: HALF-SHELL T MATRIX

After the treatment of the on-the-energy-shell quantities, we turn to the half-shell T matrix. As is well known the half-shell T matrix determines completely the two-body scattering wave function $\Psi_{\mathbf{k}}^{(+)}(\mathbf{r})$. The latter in turn determines, for instance, the probability for relaxation induced by magnetic dipole interactions in adsorbed H₁, via its role as an initial or final state in a distorted-wave Born integral. With that application in mind we specialize in this section to $n = 2$. In the restricted portion of

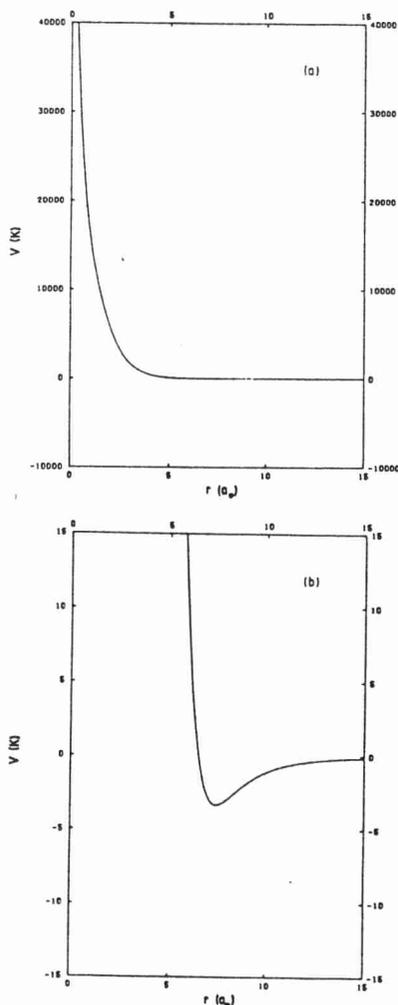


FIG. 1. (a) Potential ($2\frac{1}{2}$ -dimensional model) among two hydrogen atoms in the $|b\rangle$ state and adsorbed on the superfluid helium surface. (b) Modified version with expanded vertical scale showing the shallow potential well due to the van der Waals interaction.

space contributing effectively to the Born integral and for the relevant low collision energies $\Psi_E^{(+)}(\mathbf{r})$ is to a very good approximation rotationally symmetric and given by

$$\Psi_E^{(+)}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} \int_0^\infty dp p J_0(pr) \times \left[\frac{\delta(p-k)}{p} + \frac{1}{E^+ - p^2} T(p, k, E) \right], \quad (16)$$

in terms of the half-shell T matrix for the lowest partial wave.

$$\Psi_E^{(+)}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} \frac{1}{[1/\tau^\Lambda(k, k, E)] - I_\Lambda(E)} \left[\frac{J_0(kr)}{\tau^\Lambda(k, k, E)} + \int_0^\infty dp \frac{p}{E - p^2} \left[\frac{\tau^\Lambda(p, k, E)}{\tau^\Lambda(k, k, E)} J_0(pr) - \Theta(\Lambda - p) J_0(kr) \right] \right]. \quad (18)$$

We then take the limit $E, k \rightarrow 0$ in the expression between square brackets, which is possible because it is a smooth function of these variables. (See Sec. II.) Hence in the domain $E \ll 1/r_0^2$ (for radii $r < r_0$, $V(r)$ is significantly different from zero) and $r \ll 1/\sqrt{E}$ the wave function is well described by

$$\Psi_E^{(+)}(\mathbf{r}) = \frac{1}{[1/\tau^\Lambda(k, k, E)] - I_\Lambda(E)} \frac{\psi(r)}{\sqrt{2\pi}}, \quad (19)$$

in which the energy-independent function $\psi(r)$ is given by

$$\psi(r) = \frac{1}{\tau^\Lambda(0, 0, 0)} - \int_0^\infty \frac{dp}{p} \left[\frac{\tau^\Lambda(p, 0, 0)}{\tau^\Lambda(0, 0, 0)} J_0(pr) - \Theta(\Lambda - p) \right]. \quad (20)$$

In Fig. 2 the function $\psi(r)$ in the case of two colliding b atoms is presented. Equation (19) is in agreement with a result obtained earlier,⁹ i.e., for small E the energy dependence is given by a simple factor

$$[\pi i/2 - \ln(ka/2) - \gamma + O(k^2)]^{-1}.$$

The explicit expression (20) for $\psi(r)$ is an extension with respect to the $\ln(r/a)$ dependence outside the range of the interaction ($r > r_0$), which was found in Ref. 9.

As mentioned before, the E dependence (19) of the two-body wave function may be used to calculate the temperature dependence of magnetic dipole relaxation rates in adsorbed H \downarrow . Suppose that the energy released in the reaction is large. In that case the E dependence of the final state may be neglected at the low temperature considered. Then the temperature behavior of these two-body decay rates is governed by the factor

$$C_s(T) = \left\langle \left| \frac{1}{[1/\tau^\Lambda(k, k, E)] - I_\Lambda(E)} \right|^2 \right\rangle_{\text{th}} = \left\langle \frac{1}{\pi^2/4 + [\ln(ka/2) + \gamma + O(k^2)]^2} \right\rangle_{\text{th}}, \quad (21)$$

in which the thermal average is over the relative energy E of the colliding particles. If, on the contrary, the amount of energy released is small, such as for the process $bb \rightarrow ab$, the $l=0 \rightarrow l=0$ contribution (usually denoted by $m=0 \rightarrow m=0$) to the rate dominates and the final-state wave function also has a significant logarithmic energy dependence. Therefore the thermal average in Eq. (21) should be replaced by one over the product of two factors, both for the initial and final channels, to obtain more accurate results. Again this agrees with the conclusions of Verhaar *et al.*⁹

Another application is the recombination of three $|b\rangle$ -state hydrogen atoms adsorbed on the helium surface. In analogy to two-body scattering we can show that the exact symmetrical initial state $\Psi_E^{(+)}(\mathbf{r}, \mathbf{R})$ takes the form

$$\Psi_E^{(+)}(\mathbf{r}_1, \mathbf{R}_1) = \sum_{i=1}^3 \frac{\chi(\mathbf{r}_1, \mathbf{R}_1; \mathbf{p}_i, \mathbf{q}_i)}{[1/\tau^\Lambda(\mathbf{p}_i, \mathbf{p}_i, \mathbf{p}_i^2)] - I_\Lambda(\mathbf{p}_i^2)}, \quad (22)$$

where $\{\mathbf{p}_i, \mathbf{q}_i\}$ are the Jacobi momenta of the incoming

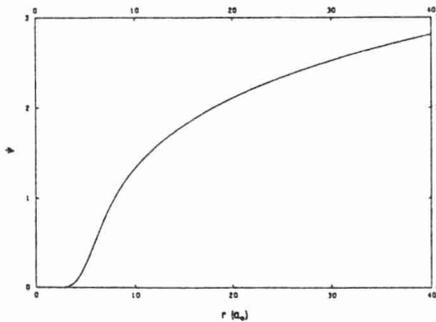


FIG. 2. The energy-independent part $\psi(r)$ of the scattering wave function of two b atoms at low energies [Eqs. (19) and (20)].

particles obeying the on-shell condition $E = p^2 + 3q^2/4$ and $\{r_i, \mathbf{R}_i\}$ stands for one of the three particular choices of Jacobi coordinates.⁵ Unfortunately the precise behavior of $\chi(\mathbf{r}, \mathbf{R}; \mathbf{p}_i, \mathbf{q}_i)$ as a function of \mathbf{p}_i and \mathbf{q}_i is difficult to analyze, because the kernel of the Faddeev equations contains singularities due to the free propagator

$$1/(E^+ - p^2 - 3q^2/4)$$

that are not damped out by phase-space factors in the limit $E \rightarrow 0$, in contrast with the three-dimensional situation.³ Furthermore, the T matrix with its logarithmic energy dependence is also involved in the kernel and may induce a strong \mathbf{p}_i and \mathbf{q}_i dependence. In view of these difficulties, it does not seem possible at present to make general statements concerning the properties of χ for small \mathbf{p}_i and \mathbf{q}_i on the basis of the Faddeev formalism.

However, such statements are possible in the context of a simple Jastrow-type ansatz for $\Psi_E^+(\mathbf{r}_1, \mathbf{R}_1)$, which has proved to be excellent for $E = 0$ in three dimensions.¹¹ Including also the center-of-mass wave function $\exp(i\mathbf{K} \cdot \mathbf{R})$ and denoting the position and momentum of particle j by \mathbf{x}_j and \mathbf{k}_j , respectively, it reads

$$\begin{aligned} e^{i\mathbf{K} \cdot \mathbf{R}} \Psi_E^+(\mathbf{r}_1, \mathbf{R}_1) = & \sum_p \mathcal{P} e^{i\mathbf{k}_1 \cdot \mathbf{x}_1} e^{i\mathbf{k}_2 \cdot \mathbf{x}_2} e^{i\mathbf{k}_3 \cdot \mathbf{x}_3} \\ & \times F_{p_1}(\mathbf{r}_1) F_{p_2}(\mathbf{r}_2) F_{p_3}(\mathbf{r}_3), \end{aligned} \quad (23)$$

where the summation is over all possible permutations of the three particles. Note that the variables \mathbf{r}_i and \mathbf{p}_i in Eq. (23), contrary to \mathbf{x}_i and \mathbf{k}_i , are numbered according to the spectator-index notation. The Jastrow factors $F_p(\mathbf{r})$ tend to 1 for large separations and depend on the asymptotic relative momenta among the particles. They are of such a form that the \mathbf{r}_i part of Ψ_E^+ , i.e.,

$$e^{i\mathbf{p}_i \cdot \mathbf{r}_i} F_{p_i}(\mathbf{r}_i) \equiv G_{p_i}(\mathbf{r}_i)$$

is identical to a two-body scattering state. Applying this same idea in two dimensions we have [cf. Eq. (19)]

$$G_p(\mathbf{r}) = \frac{1}{[1/\tau^\Lambda(p, p, p^2)] - I_\Lambda(p^2)} \frac{\psi(\mathbf{r})}{\sqrt{2\pi}}. \quad (24)$$

Thus the wave function (23) becomes a product of three G functions multiplied by an exponential. In the low-temperature limit the latter can be replaced by 1, the dominant energy dependence being contained in the product

$$\prod_{i=1}^3 \frac{1}{[1/\tau^\Lambda(p_i, p_i, p_i^2)] - I_\Lambda(p_i^2)}.$$

The behavior at low temperatures of, for instance, a three-body recombination decay rate is therefore given by a Boltzmann average of this quantity, which can be evaluated readily without detailed knowledge of the wave function $\Psi_E^+(\mathbf{r}_1, \mathbf{R}_1)$.

V. SEPARABLE APPROXIMATION TO THE T MATRIX

In this section we will only consider three dimensions, although the discussions can immediately be generalized

to arbitrary dimension. In the context of three-body calculations it is favorable to dispose of separable expressions for the two-body T matrix. As is well known the Faddeev equations then reduce to a two-body problem. Our aim is to find such a separable approximation by neglecting the $\tau^\Lambda(p, p', E)$ term in the right-hand side of Eq. (7) that contains Λ as a free parameter. Minimizing this term, in a certain sense, as a function of Λ , one might hope that the separable part

$$\begin{aligned} T^{SA}(p, p', E) = & \frac{\tau^\Lambda(p, k, E) \tau^\Lambda(k, p', E)}{\tau^\Lambda(k, k, E)} \\ & \times \left[\frac{1}{1 - I_\Lambda(E) \tau^\Lambda(k, k, E)} - 1 \right] \end{aligned} \quad (25)$$

of the right-hand side constitutes an accurate approximation to the T matrix. Neglecting the -1 term one would be led to the separable expression obtained by using the Noyes-Kowalski method.¹² As is well known this term has unphysical poles whenever the on-shell T -matrix element $T(k, k, E)$, or equivalently $\tau^\Lambda(k, k, E)$, is equal to zero. In our case they are canceled by including the -1 term. Actually, it was already shown by Osborn¹³ that such a pole could be avoided by adding an additional separable term to the approximation. Because his method involves the eigenfunctions of the Noyes-Kowalski kernel, it is rather laborious in contrast with our method, where only the τ^Λ matrix is needed. A second advantage of our approach is connected with the possibility of applying it to negative energies, which are unavoidable in three-body calculations; Eq. (25) can be used for both signs of E if we define for example $k^2 = |E|$. Actually, if $E < 0$ any k can be used, because in this case the integrand of Eq. (4) contains no singularities. We thus do not need to solve integral equations as in the Noyes-Kowalski method, where the V matrix for complex momenta is required with all associated complications in the case of long-range potentials (like the van der Waals interaction decaying as $1/r^6$).

It is also possible to find a connection with the W matrix of Bartnik *et al.*¹⁴ The W matrix too has the important disadvantage that it does not contain a free parameter, making it impossible to optimize the separable approximation. One is therefore completely dependent on the specific features of the potential which should make the remaining nonseparable part sufficiently small.

One way to optimize our separable approximation would be by minimizing the norm squared of the neglected τ term,

$$\|\tau\|^2 = \int d\mu(p) \int d\mu(p') \tau^2(p, p', E) \equiv (\tau, \tau) \quad (26)$$

using some measure $\mu(p)$ to evaluate the integrals involved. For example, the measure $\mu(p) = p^n/n$ results in the usual Hilbert-Schmidt norm, since the τ matrix is real and symmetric in the momentum variables. Actually, the choice of $\mu(p)$ is a second degree of freedom in addition to the value of Λ , to optimize the separable approximation; it can be used to emphasize specific regions of the (p, p') plane where the approximation should be accurate. To find an algorithm for actual calculations that accomplishes the minimalization, we recall that the matrices

$$A(p, p', E) = \frac{\tau^\Lambda(p, k, E) \tau^\Lambda(k, p', E)}{[\tau^\Lambda(k, k, E)]^2},$$

$$B(p, p', E) = \tau^\Lambda(p, p', E) - A(p, p', E) \tau^\Lambda(k, k, E) \quad (27)$$

are independent of Λ . Expressing $\tau^\Lambda(p, p', E)$ in terms of $A(p, p', E)$, $B(p, p', E)$, and the matrix element $\tau^\Lambda(k, k, E)$, the condition $\partial \|\tau^\Lambda\|^2 / \partial \Lambda = 0$ amounts to

$$\tau^\Lambda(k, k, E) = - \frac{(A(E), B(E))}{(A(E), A(E))}, \quad (28)$$

where we denote the optimal choice of the cutoff parameter by Λ' .

Summarizing, the algorithm runs as follows.

- (1) Choose a $\Lambda > k$ and calculate $\tau^\Lambda(p, p', E)$.
- (2) Determine the matrices $A(p, p', E)$ and $B(p, p', E)$, which are independent of Λ .
- (3) Find the optimal on-shell matrix element $\tau^{\Lambda'}(k, k, E)$ determined by Eq. (28).
- (4) Use the matrices A and B to obtain $\tau^{\Lambda'}(p, p', E)$ and Eq. (25) to find the optimal separable approximation.

As an example of this procedure we consider nucleon-nucleon scattering using the Malfliet-Tjon III potential.¹⁵ We use the convenient measure $\mu(p) = \ln(p)$ to stress small momenta where the T matrix is large. In Fig. 3 we present the V matrix, the exact T matrix at an energy of 1 MeV, our optimized separable approximation T^{SA} and

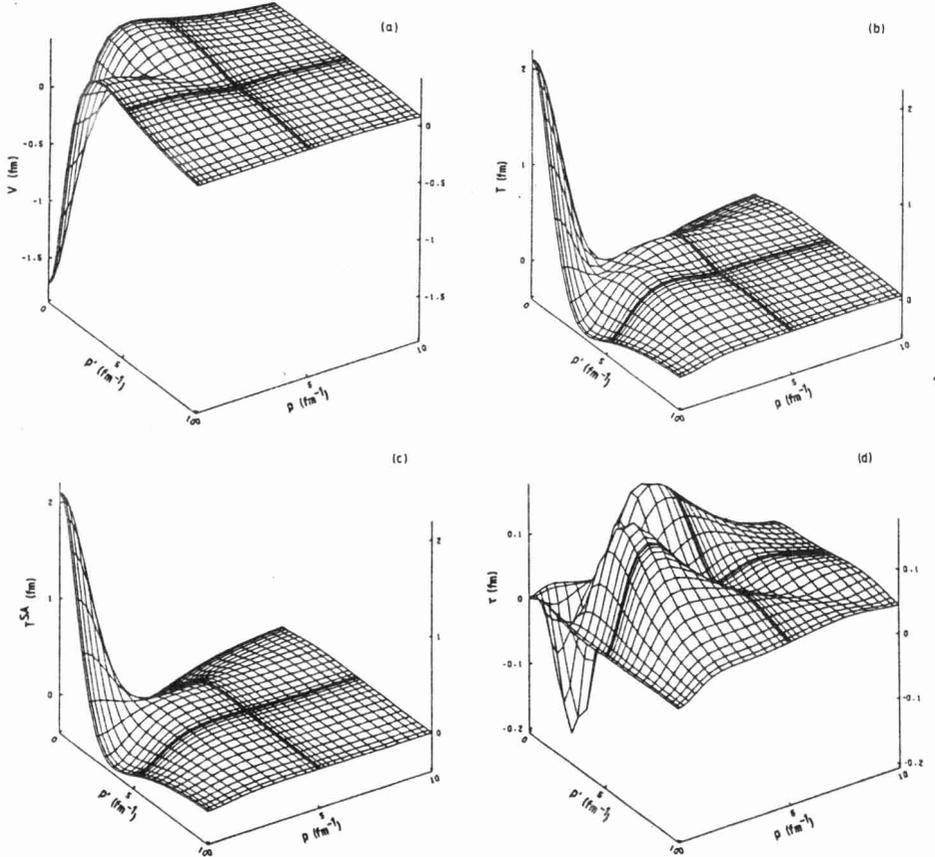


FIG. 3. Illustration of the accuracy of the separable approximation T^{SA} in the case of a Malfliet-Tjon III potential and a total angular momentum $l=0$. (a) Potential surface $V(p, p')$. (b) Exact T matrix at an energy of 1 MeV. (c) Separable approximation T^{SA} obtained by using the measure $\mu(p) = \ln(p)$ in the optimization procedure and (d) the τ^Λ matrix representing the difference between T and T^{SA} .

τ^Λ , i.e., the difference between T and T^{SA} . Apparently, the latter is relatively small in the part of the (p, p') plane where the T matrix is large. Furthermore, we note that in this way the unphysical poles in the τ^Λ matrix, which are introduced because Λ is finite, are always avoided because the norm $\|\tau^\Lambda(E)\|$ would else be infinite.

Finally, we would like to point to the huge amount of freedom available to improve in particular on the last comparison by extending the τ method in a similar way as proposed by Adhikari;¹⁶ the function $\Theta(\Lambda - p')$ in Eq. (4) defining τ^Λ can in principle be replaced by any function with the value 1 for $p' = k$ without invalidating the method. Note, however, that the approaches still differ. Our proposal leads to an explicit energy dependence of all scattering observables, without resorting to Jost functions which have to be evaluated numerically. It would be interesting to find out to what extent further improvements of the separable approximation may be achieved in this way.

VI. CONCLUSIONS

Summarizing, we recall that the nonsingular equation for the τ matrix is numerically easy to handle and has a solution that is well behaved close to the energy $E=0$. Due to this feature the τ matrix can be used to formulate an effective-range theory in arbitrary dimension and to find the (small- E) energy dependence of all kinds of important scattering quantities, such as the wave function and the phase shift.

In the context of three-body calculations, the method introduced may be useful for analyzing the singularities involved in the kernel of the Faddeev equation for three asymptotically free particles and to find a satisfactory separable approximation to the T matrix that avoids unphysical poles and is applicable to negative energies.

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APPENDIX

In this appendix we study the behavior of the τ^Λ matrix as a function of the momentum and energy variables in the special situation of $n=2$ and $l=0$, which is the most important case with respect to applications in the context of low-energy scattering. Moreover, we will prove that $\tau^\Lambda(p, p', E)$ and also its on- and half-shell counterparts are well-behaved functions of energy, with an asymptotic expansion for $E \downarrow 0$.

Studying the E dependence by means of Eq. (4) is not very convenient, because it is not an integral equation of the Fredholm type. To avoid this problem we introduce a new matrix $\rho^\Lambda(p, p', E)$, which is defined by

$$\rho^\Lambda(p, p', E) = V(p, p') + \int_0^\infty dp'' \frac{p''}{E - (p'')^2} \left[V(p, p'') - \Theta(\Lambda - p'') \frac{V(p, k)V(k, p'')}{V(k, k)} \right] \rho^\Lambda(p'', p', E) \quad (A1)$$

and in terms of which $\tau^\Lambda(p, p', E)$ can be expressed as

$$\tau^\Lambda(p, p', E) = \rho^\Lambda(p, p', E) - \frac{\rho^\Lambda(p, k, E) \int_0^\Lambda dp'' \frac{p''}{E - (p'')^2} [V(k, k)\rho^\Lambda(k, p', E) - V(k, p'')\rho^\Lambda(p'', p', E)]}{V(k, k) + \int_0^\Lambda dp'' \frac{p''}{E - (p'')^2} [V(k, k)\rho^\Lambda(k, k, E) - V(k, p'')\rho^\Lambda(p'', k, E)]} \quad (A2)$$

Due to the last relation, which involves only proper integrals with regular integrand, τ^Λ is found to be a well-behaved function of energy with an asymptotic expansion for $E \downarrow 0$, if the same is true for the dependence of the ρ^Λ matrix on all its arguments. We start by considering the explicit energy dependence and return to the problem associated with the momentum variables later on.

We consider Eq. (A1) as a problem in the Hilbert space $L_2(\mathbb{R}^+)$ of the p variable and rewrite it in an abstract notation,

$$|\rho^\Lambda(p', E)\rangle = |V(p')\rangle + K_\Lambda(E) |\rho^\Lambda(p', E)\rangle, \quad (A3)$$

where we explicitly show the special role of p' as a dummy variable, which plays no role in the integral equation itself. Note that the phase-space factor p'' in Eq. (A1) is included in $K_\Lambda(E)$.

Our proof is now based on the following theorem. If (i) $K_\Lambda(E)$ is bounded for $0 \leq E < \epsilon$; (ii) $[1 - K_\Lambda(E)]^{-1}$ exists

for $0 \leq E < \epsilon$, which means that 1 should not be in the spectrum of $K_\Lambda(E)$; and (iii) $K_\Lambda(E)$ has an asymptotic expansion,

$$K_\Lambda(E) = \sum_{i=0}^m K_i^\Lambda E^i + R_\Lambda(E), \quad (A4)$$

$$\lim_{E \downarrow 0} \|R_\Lambda(E)\|/E^m = 0,$$

with bounded operators K_i^Λ , then Eq. (A3) has a solution in $L_2(\mathbb{R}^+)$ equal to $[1 - K_\Lambda(E)]^{-1} |V(p')\rangle$ having an asymptotic expansion given by

$$|\rho^\Lambda(p', E)\rangle = \sum_{i=0}^m E^i |\rho_i^\Lambda(p')\rangle + |\sigma^\Lambda(p', E)\rangle, \quad (A5)$$

$$\lim_{E \downarrow 0} \|\sigma^\Lambda(p', E)\|/E^m = 0.$$

Here $\|O\|$ is the usual notation for the norm of the opera-

for O . The theorem is easily proved by using the resolvent identity

$$\begin{aligned}
 [1 - K_\Lambda(E)]^{-1} &= (1 - K_0^\Lambda)^{-1} \\
 &+ (1 - K_0^\Lambda)^{-1} \left[\sum_{i=1}^m K_i^\Lambda E^i + R_\Lambda(E) \right] \\
 &\times [1 - K_\Lambda(E)]^{-1} \tag{A6}
 \end{aligned}$$

and substituting it into

$$|\rho^\Lambda(p', E)\rangle = [1 - K_\Lambda(E)]^{-1} |V(p')\rangle$$

to find the equation

$$\begin{aligned}
 |\rho^\Lambda(p', E)\rangle &= (1 - K_0^\Lambda)^{-1} |V(p')\rangle \\
 &+ (1 - K_0^\Lambda)^{-1} \left[\sum_{i=0}^m K_i^\Lambda E^i + R_\Lambda(E) \right] \\
 &\times |\rho^\Lambda(p', E)\rangle.
 \end{aligned}$$

Iterating m times leads to an asymptotic expansion of the form given by Eq. (A5), because all vectors and operators involved are bounded due to the assumptions of the theorem.

Furthermore, if $K_\Lambda(E)$ is bounded, if $|V(p')\rangle$ has an asymptotic expansion that is schematically denoted by

$$|V(p')\rangle \underset{p'^{10}}{\sim} \sum_{i=1}^m (p')^{2i} |V_{2i}\rangle + o((p')^{2m}),$$

and if all the vectors $|V_{2i}\rangle$ are elements of $L_2(\mathbb{R}^+)$, then we find by substituting this expansion into the formal solution of Eq. (A3) that $|\rho^\Lambda(p', E)\rangle$ has a similar asymptotic expansion in p^2 for $p' \downarrow 0$.

To complete the discussion about the energy and momentum dependence of $\rho^\Lambda(p, p', E)$, we will now show that for a realistic potential $V(r)$ the requirements of the above theorems are fulfilled. The transformation to momentum space of the potential ($n=2$ and $l=0$) is given by

$$\bar{V}(Q) = \int_0^\infty dr r V(r) J_0(Qr), \tag{A7}$$

$$V(p, p') = \frac{1}{2\pi} \int_0^{2\pi} d\phi \bar{V}[(p^2 + p'^2 - 2pp' \cos\phi)^{1/2}].$$

The lemma of Riemann-Lebesgue¹⁷ states that $\bar{V}(Q) \sim o(1/\sqrt{Q})$ as $Q \rightarrow \infty$, if $V(r)$ is continuous and the integral

$$\int_0^\infty dr \sqrt{r} V(r)$$

is absolutely convergent. In particular, the potential of the $2\frac{1}{2}$ -dimensional model (Fig. 1) behaving as $-\ln(r)$ for small r and r^{-6} for large r , obeys these conditions. Because $\bar{V}(Q)$ exists for every $Q \geq 0$ we can formulate the following upper bound with a proper positive value for μ :

$$|\bar{V}(Q)| \leq \frac{C}{(1+Q)^{1/2+\mu}}, \tag{A8}$$

and therefore also

$$|V(p, p')| \leq \frac{C}{(1+|p-p'|)^{1/2+\mu}}, \tag{A9}$$

which is sufficient to show that $|V(p')\rangle$ is indeed for all p' an element of the Hilbert space $L_2(\mathbb{R}^+)$. To show that the kernel is bounded we look at the Hilbert-Schmidt norm $\|K_\Lambda(E)\|_{\text{HS}}$. As in the treatment of Osborn¹³ we write the norm squared as the sum of terms $L_\Lambda(E)$ and $M_\Lambda(E)$,

$$L_\Lambda(E) = \int_0^\infty dp \int_{k+1}^\infty dp' |K_\Lambda(p, p', E)|^2,$$

$$M_\Lambda(E) = \int_0^\infty dp \int_0^{k+1} dp' |K_\Lambda(p, p', E)|^2.$$

Furthermore, because of our interest in low-energy scattering we assume for simplicity $0 \leq E < \epsilon < 1$.

Using Eq. (A9) we find that $L_\Lambda(E) < \infty$, but to analyze $M_\Lambda(E)$ we need the smoothness condition

$$|V(p + \Delta p, p') - V(p, p')| \leq \frac{C' |\Delta p|}{(1+|p-p'|)^{3/2+\mu}}, \tag{A10}$$

because of the pole involved in the integration over p' . This condition is easily derived by applying the mean value theorem and using

$$\left| \frac{\partial V(p, p')}{\partial p} \right| \leq \frac{C'}{(1+|p-p'|)^{3/2+\mu}}, \tag{A11}$$

for $V(r)$ obeying the requirements of the Riemann-Lebesgue theorem. On the basis of Eq. (A10) we can now show that $M_\Lambda(E)$ is finite and therefore that the operator $K_\Lambda(E)$ is bounded.

Finally, we need to consider the operators

$$K_i^\Lambda \equiv \frac{1}{i!} \frac{d^i K_\Lambda(E)}{dE^i} \Big|_{E=0}$$

and the vectors

$$|V_i\rangle \equiv \frac{1}{i!} \frac{d^i |V(p')\rangle}{dp'^i} \Big|_{p'=0}$$

The problem for $K_0^\Lambda = K_\Lambda(0)$ and $|V_0\rangle = |V(0)\rangle$ has already been solved, but in the case of $i > 0$ the partial derivatives $\partial^i V(p, p') / \partial p'^i |_{p'=0}$ come into play. They have the upper bound

$$\left| \frac{\partial^i V(p, p')}{\partial p'^i} \Big|_{p'=0} \right| \leq \frac{C_i}{(1+p')^{i+1/2+\mu}}, \tag{A12}$$

with $C_i = 0$ for odd i . This leads to the conclusion that $K_i^\Lambda(p, p')$ decreases for large p and p' at least as fast as $K_0^\Lambda(p, p')$. Because of this and the fact that $K_i^\Lambda(p, p')$ contains no poles its Hilbert-Schmidt norm exists, so that the operator K_i^Λ is bounded. In addition, Eq. (A12) is sufficient to prove that also the norm of $|V_i\rangle$ is finite.

Summarizing, we have shown that $\rho^\Lambda(p, p', E)$ and therefore $\tau^\Lambda(p, p', E)$ is a well-behaved function of energy and momentum, with an asymptotic expansion for $E \downarrow 0$. This has also been shown to be true for the on- and half-

shell τ -matrix elements. Our conclusion, formulated in Sec. II, that the singular energy dependence of the T matrix is concentrated in the function $I_\Lambda(E)$ is therefore justified.

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CHAPTER 6:
SPIN-POLARIZED ATOMIC HYDROGEN
IN VERY STRONG MAGNETIC FIELDS

Spin-polarized atomic hydrogen in very strong magnetic fields

H. T. C. Stoof, L. P. H. de Goey, and B. J. Verhaar

Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

W. Glöckle

Institut für Theoretische Physik, Ruhr Universität Bochum, Bochum, Federal Republic of Germany

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We calculate the effective rate constant for three-body dipolar recombination of spin-polarized atomic hydrogen in conditions of high density and very high magnetic field strengths (beyond the <10-T range of previous calculations). We find that the decay of the gas sample is not sufficiently suppressed at magnetic fields available in the foreseeable future.

I. INTRODUCTION

In the past several years intense experimental efforts have been going on to produce atomic hydrogen in a state of Bose-Einstein condensation (BEC), all of which have been thwarted by the presence of a rather large rate for recombination into a molecular state via three-body collisions.¹ In one of the experiments, for instance, the highest density achieved at $T=550$ mK was 4.5×10^{18} cm^{-3} , an order of magnitude lower than the critical density at this temperature. Various ingenious schemes have been proposed to avoid this problem: wall-free confinement of the hydrogen atoms,² or more recently the possibility of applying microwave cooling to lower the temperature and thus lower the densities needed to arrive at the condensation regime.³

Another line of investigation continues the high-density approach, but aims at suppressing the three-body recombination by substantially increasing the magnetic field above values used in earlier studies.⁴ Simple models^{5,6,7} predict the decay of the gas to fall sharply at $B \approx 27$ T and at $B \approx 54$ T. More recent calculations⁸ for fields $B < 10$ T, relaxing some of the rough approximations in the earlier simple models, led to considerable corrections in this lower field range. It is therefore of interest to see whether minima at 27 or 54 T might be even lower on the basis of our more exact method, so as to be promising from the point of view of reaching BEC. The purpose of the present paper is to extend these calculations to higher fields. Our main conclusion is that recombination is not sufficiently suppressed at magnetic fields achievable in the foreseeable future: small enough rates occur only at magnetic fields as strong as 140 T.

In the following sections we shall describe our method of calculation and its results, followed by our interpretation of the main features and some conclusions.

II. METHOD

In the zero-temperature limit and to first order in the (electron-electron) magnetic-dipole part V_{ij}^d of the H-H interaction, the three-body rate constant is given by⁷

$$L_g = \frac{(2\pi)^2 \hbar^3 m_H}{9} \sum_f q_f \int d\mathbf{q}_f \left| \langle \Psi_f^{(-)} | \sum_{i,j} V_{ij}^d | \mathcal{S}\Psi_i^{(+)} \rangle \right|^2, \quad (1)$$

where m_H is the hydrogen mass and the summation is over all possible ortho- H_2 states that can be formed on the basis of energy conservation. Furthermore, the fully symmetrized initial state $|\mathcal{S}\Psi_i^{(+)}\rangle$ is associated with the scattering of three incoming electron spin-down H atoms, while the final state $|\Psi_f^{(-)}\rangle$ describes the time reversed collision of an atom (electron spin up or down) with a molecule with relative momentum \mathbf{q}_f . Both states are normalized as in Ref. 7 and obey the three-particle Schrödinger equation with all central (singlet or triplet) interactions between the atoms included. Depending on the above-mentioned spin orientation of the final single atom parallel or antiparallel to \mathbf{B} , L_g is usually indicated as a single or double spin flip rate. Assuming the spin-flipped (SF) atom to recombine rapidly upon collision with an electron spin down atom,¹ the effective rate constant is

$$L_g^{\text{eff}}(B) = L_g^{\text{1SF}}(B) + 2L_g^{\text{2SF}}(B), \quad (2)$$

$$L_g^{\text{2SF}}(B) = 4L_g^{\text{1SF}}(2B).$$

In order to facilitate the analysis of experiments under less restrictive assumptions we present in Sec. III not only results for L_g^{eff} , but also for the ratio $L_g^{\text{2SF}}/(L_g^{\text{1SF}} + L_g^{\text{2SF}})$, i.e., the probability that after a three-body event the outgoing atom has electron spin up. Our calculation is based on the zero-temperature limit, since the bulk recombination rate is expected to have a weak temperature dependence. In the context of a zero temperature calculation, L_g^{eff} is also the effective rate constant for the dipolar part of *abb*, *aab*, and *aaa* recombination.

The initial state $|\mathcal{S}\Psi_i^{(+)}\rangle$ in Eq. (1) is calculated using an exact Faddeev-like approach.⁸ The exact calculation of the final state $|\Psi_f^{(-)}\rangle$ is practically impossible with

present computer capacities. Kagan⁵ used a plane-wave description for the relative atom-molecule motion. We use a method in which all (in)elastic atom-molecule interactions are taken into account, but we neglect rearrangement of atoms. The latter appears to be essential to describe the three-body process at lower fields (the so-called dipole-exchange mechanism^{6,7}), but on the basis of simple models⁷ is expected to fall off rapidly with increasing field.

To be more precise about the approximations involved in the final state we give a short summary, referring to

$$\left[\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + \frac{\lambda(\lambda+1)\hbar^2}{2\mu R^2} + V_{vj\lambda, v'j'\lambda}^{L\pi}(R) + \epsilon_{vj} - E \right] f_{vj\lambda}^{L\pi}(R) = - \sum_{v'j'\lambda'} V_{vj\lambda, v'j'\lambda'}^{L\pi}(R) f_{v'j'\lambda'}^{L\pi}(R) \quad (3)$$

for the relative motion with reduced mass $\mu = 2m_H/3$ and rotation-vibration energy ϵ_{vj} . For each fixed L and parity π the potential $V^{L\pi}$ couples all channels obeying $|j-L| \leq \lambda \leq j+L$ with j odd and $(-1)^\lambda = -\pi$.

After a transformation to a momentum space Lippmann-Schwinger equation and a numerical discretization, the solution is found by matrix inversion. To obtain a converged result for the rate constant L_g^{eff} we had to include all rotational levels belonging to the $v=13$ and 14 vibrational levels. Hence a total of 16 channels are involved in the calculation although only the final states $|\Psi_f^{(-)}\rangle$ corresponding to the $(v,j)=(14,1)$, $(14,3)$ and $(13,5)$ outgoing channels contribute substantially to the rate in the magnetic-field range studied.

III. RESULTS

In Figs. 1 and 2 we present our results for L_g^{eff} and compare with the Kagan model. In addition, the single and double spin-flip field ranges have been indicated for the $(14,3)$ and $(14,1)$ molecular states. In Fig. 1 we clearly see the repetitive structure as a function of B . The $(14,3)$ double spin-flip maximum around 15 T is followed by a

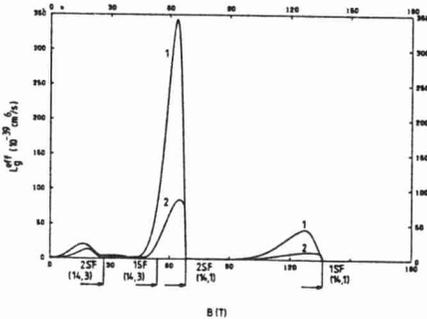


FIG. 1. Effective decay rate L_g^{eff} as a function of the applied magnetic field [(1) Kagan's model and (2) this work]. Also indicated are the single and double spin-flip cutoff fields for the bound states $(14,3)$ and $(14,1)$.

Ref. 8 for a more extensive treatment.⁹ In a time-reversed picture the atom collides with a molecule in an excited rotation-vibration state (at lower magnetic fields primarily the $v=14, j=3$ state) and (de)excites it during the collision to, in principle, all other (v,j) states. Whereas the total orbital angular momentum L of the three-body system is conserved, the relative orbital angular momentum λ between the single atom and molecule can change, the interaction being anisotropic. This results in the (coupled-channels) Schrödinger equation

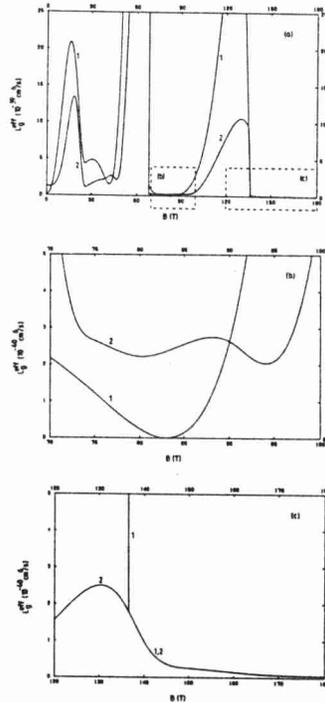


FIG. 2. A more detailed study of the magnetic field dependence of L_g^{eff} : (a) Shows L_g^{eff} on an expanded vertical scale, which displays more clearly the complicated structure of the rate constant in the case of (1) Kagan's model and (2) our approach. (b) An enlargement of the region around 83 T, where the Kagan model predicts the rate constant to be zero. This zero is removed in our calculations. (c) Shows the region beyond the single spin-flip cutoff of the $(14,1)$ bound state [(1): The decay rate L_g^{eff} and (2): the partial contribution from the $(13,5)$ bound state]. For magnetic fields $B > 136.4$ T Kagan's rate constant is negligible and invisible on this scale.

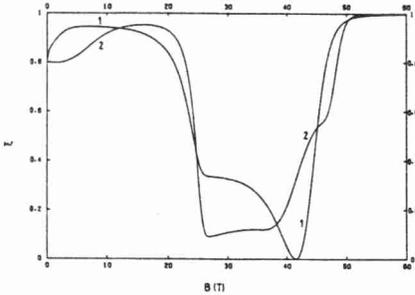


FIG. 3. The probability ξ for a double spin-flip event as a function of magnetic field [(1) Kagan's model and (2) this work].

lower single spin-flip maximum at about 30 T. A more pronounced (14,1) double spin-flip peak near 60 T is followed by a less pronounced single spin-flip peak near 120 T. Note the strong formation probability of the (14,1) state for B smaller than 68.2 T. The (14,3) maxima are much lower due to the higher rotational angular momentum that the dipolar interaction has to introduce into a two-atom subsystem starting from a situation of vanishing relative orbital angular momenta in the initial state.

A general feature, evident from the behavior of L_g^{eff} , is the decrease of our values compared to Kagan's by a factor of about 3, especially on the low- B side of each of the maxima. This is due to the inclusion of correlations between the particles in both the initial and final states. These correlations cause the three-body wave function to be zero in all parts of configuration space where two or three atoms are close together and therefore reduce the transition probability. Clearly, the reduction is expected to be less on the high- B , i.e., low- q_f side: the centrifugal barrier in the final channel then by itself already keeps the final atom out of the forbidden region. Hence the Kagan model should then be an excellent approximation. This is indeed borne out by our calculations. In particular, the partial (v, j) contributions to L_g^{eff} show the $(B_0 - B)^{j+1/2}$ behavior on the high- B side of each of the maxima, that also follows from the Kagan approach. It should be noted, however, that from the point of view of BEC one is more interested in B values where L_g^{eff} is small. There the deviations from Kagan's model are considerable. Close to 27 T the rate is relatively small, but not small enough to be promising. At 83 T the Kagan (14,1) rate goes through zero. This potentially interesting B value is unfortunately eliminated by our calculation [see Fig. 2(b)]. The decay time of the atomic density due to recombination varying with n_H^2 , an increase of the density by a factor of 10 with respect to the above-mentioned experiment,¹ would require L_g^{eff} to be as small as 10^{-40} cm⁶/s. It follows from Fig. 2(c) that such values occur only above 140 T. Notwithstanding the recent develop-

ments with respect to high- T_c superconductivity,¹⁰ this field region is practically of little importance in the foreseeable future. Nevertheless, from the point of view of interaction mechanisms it is interesting to point out that the Kagan model predicts a negligible rate beyond 136.4 T. This is indeed what one would expect in the first instance, because the only possible final H_2 states in that region are the more strongly bound $v=13$ states. Figure 2(c) shows, however, larger L_g^{eff} values according to our calculations, due to indirect population of the (13,5) state via a strong coupling to the closed (14,1) channel which, as pointed out above, are strongly populated directly from the initial state.

For experimental purposes we also give in Fig. 3 the ratio between $L_g^{2\text{SF}}$ and $L_g^{1\text{SF}} + L_g^{2\text{SF}}$, denoted by ξ . This quantity is of importance in the analysis of the experimental data, if one wants to include the possibility of relaxation of the electron spin-up atom that is produced in the double spin-flip process. As previously noted, we neglect this possibility in the definition of L_g^{eff} and assume that the $|c\rangle$ or $|d\rangle$ atom recombines with an $|a\rangle$ or $|b\rangle$ state particle on the helium surface. We find that the field dependence of ξ is almost linear in the range $5\text{T} \leq B \leq 10\text{T}$, where most of the experiments until now have been carried out. In this range Kagan predicts ξ to be a constant equal to 0.93. Experimentally this value is always used to describe the decay of the gas sample due to three-body recombination.^{1,11}

IV. CONCLUSIONS

We have studied the prospects for producing atomic hydrogen in a state of Bose-Einstein condensation at high magnetic fields, where the effects of rearrangement (the dipole-exchange mechanism) are expected to be negligible. The calculations include all three-atom correlations in the spin-polarized initial state, as well as the elastic and inelastic distortions of the atom plus molecule final state. The single and double spin flip bumps in a partial (v, j) contribution to the rate constant show agreement with Kagan's model at the high- B (low- q_f) slope, due to the centrifugal effect. At the low- B (high- q_f) slope our values are smaller by a factor of about 3. From the point of view of BEC, ranges of B with a small rate value are of importance. There the relative deviations from Kagan are considerable. Despite the difference no sufficiently small rate is found near 27 T and 54 T. A zero L_g^{eff} value at about 83 T according to Kagan's model turns into a too large rate constant on the basis of our calculation. Recombination is sufficiently suppressed only at fields stronger than 140 T.

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CHAPTER 7:
RESONANCES IN RECOMBINATION OF ATOMIC HYDROGEN
DUE TO LONGE-RANGE H_3 MOLECULAR STATES

Resonances in recombination of atomic hydrogen
due to long-range H_3 molecular states

H.T.C. Stoof, B.J. Verhaar, and L.P.H. de Coey
*Department of Physics, Eindhoven University of Technology,
5600 MB Eindhoven, The Netherlands.*

W. Glöckle
*Institut für Theoretische Physik, Ruhr Universität Bochum,
Bochum, Federal Republic of Germany.*

We present a calculation of the effective rate constant for three-body recombination, taking for the first time rearrangement into account. We find a pronounced resonance structure as a function of magnetic field due to long-range rovibrational states of H_3 in an almost equilateral configuration. This structure is superposed on a rather flat background with a slow decrease below 10T. The results are compared with experiment.

I. INTRODUCTION

A vital and still actual question in the field of spin-polarized atomic hydrogen is: Will the finite lifetime due to collisional processes be longer than the time required for the establishment of the Bose condensed state? Theoretically this problem is far from settled and experimentally one has still not been able to reach a definitive conclusion, the present situation being that both the low and high density schemes, using traps^{1,2} or compression of hydrogen bubbles³ respectively, are plagued by large decay rates.

However, to arrive at the Bose condensation regime, the density and hence the number of collisions per unit time may be kept at an acceptable minimum if one is able to cool the trapped atoms sufficiently or to affect directly the decay constants, which govern the time evolution of the system. The former goal may be achieved by using for instance evaporative¹ or laser (Lyman- α) cooling,⁴ whereas the rate constants can be manipulated by a variation of external parameters such as the detuning of a microwave trap⁵ or the applied magnetic field.

The last possibility is especially suited for the high density scheme and has stimulated the study of the three-body (dipolar) recombination process at very high field strengths both experimentally⁶ as well as theoretically.⁷ The first theoretical study⁸ of the dipolar mechanism was a breakthrough in the understanding of the properties of doubly polarized atomic hydrogen gas at high densities. However, the analytic treatment showed a strong discrepancy with the experimental field dependence below 10T. In view of the fact that the interest concentrates on values of the magnetic field for which the recombination rate is small, it is of importance to develop a more detailed picture of the recombination process. From the start the role of spin-exchange taking place after the dipole transition was recognized as an important effect: the dipole-exchange mechanism.⁹ This mechanism is contained in the f_2^d amplitude of Ref. 8, which was considered negligible in that investigation. An exact evaluation¹⁰ of the f_1^d amplitude confirmed that this part alone does not explain the recombination rate below 10T. Also, a model which takes into account (in)elastic atom-molecule scattering with a fixed bound pair and symmetrizes afterwards was unsuccessful,^{7,10} in agreement with the fact that dipole-exchange can only be included by allowing all pairs to be bound. The most recent indication that such a model is indeed unsuccessful comes from a comparison of the above-mentioned experimental and theoretical work in Refs. 6 and 7.

In the present paper we present a calculation which includes dipole-exchange in an approximate way. As we will show, this approach provides for a qualitative explanation of the slowly decreasing field dependence below 10T and in addition suggests that the high rates found in recent high-field measurements may be due to a resonance effect caused by quasi-bound $S=\frac{1}{2}$ states of the H_3 molecule. In the picture we propose, the resonance effect enhances the dipole-exchange mechanism at certain values of the final atomic kinetic energy, i.e. at certain B values.

The paper is organized as follows. In Sec. II we indicate how the rearrangement channels can be included, extending our previous calculations^{10,7} of (in)elastic atom-molecule scattering in such a way that all particle pairs are treated symmetrically from the beginning. In Sec. IIIA we give the results of the numerical evaluation of the model: We present the recombination rate constant in the magnetic field range 0-40T and extract some information on the rovibrational relaxation of highly excited H_2 molecules, which is of interest in its own right because it is to a large extent responsible for the undesirable heat-up of the gas sample. The pronounced resonance structure which shows up in the decay rate is explained in Sec. IIIB in terms of quasi-bound rovibrational states of H_3 . We end with some conclusions and suggestions for a better description of these states.

II. RESONATING-GROUP THEORY

To make the paper self-contained and to set up a convenient notation, we briefly summarize some well-known^{11,7} facts about the bulk three-body recombination constant L_g . Two-body relaxation calculations¹² have shown that it is sufficiently accurate to treat the magnetic dipole interaction as a first order perturbation. In addition, without the typical logarithmic energy dependence which prevails in two dimensions and because the highest excited states of H_2 have at least a binding energy of 70K the rate constant is expected to vary very slowly in the experimentally accessible temperature range of T<1K. Hence it is permitted to take the zero-temperature limit.

Within the framework of these approximations L_g reduces essentially to a squared matrix element of the (electron-electron) magnetic dipole interaction between symmetrized initial and final states, denoted by $|\mathcal{V}_i^{(+)}\rangle$ and $|\mathcal{V}_f^{(-)}\rangle$, respectively, summed over all possible final states. To aid physical insight we point out that the complex conjugated (i.e. time-reversed) configuration space wavefunction $\mathcal{V}_f^{(-)*}$ describes an atom-molecule collision. In terms of single and double spin-flip (SF) processes the effective rate constant becomes

$$L_g^{\text{eff}}(B) = L_g^{1SF}(B) + 2L_g^{2SF}(B) , \quad (1)$$

where we assume an additional recombination event on the helium surface after a double spin-flip process, because the outgoing atom will be in a $|c\rangle$ state.

Both initial and final states are eigenstates of the Hamiltonian

$$H = H_0 + V , \quad (2)$$

which includes the central (singlet or triplet) interactions between the hydrogen atoms. Using the spectator-index notation¹³ we write

$$V = \sum_{\alpha} V_{\alpha} \equiv V_{\alpha} + V^{\alpha} \quad (3)$$

and define the channel Hamiltonian

$$H_{\alpha} = H_0 + V_{\alpha} . \quad (4)$$

The operator H_0 is the sum of the kinetic energies in the center of mass system and the Zeeman energies of the three atoms. Note that we neglect the possibility of a three-body force, which appears justified since in the initial state all particle

pairs experience a strongly repulsive triplet interaction, while in the final state the molecular states involved, turn out to be highly excited. In both cases at least one pair has a large separation. Furthermore, the influence of the hyperfine interaction is neglected in the final state, being a small higher-order effect.

In Refs. 9 and 10 we obtained the exact initial state $|\mathcal{A}\Psi_i^{(+)}\rangle$ of three incoming spin-polarized hydrogen atoms, using the Faddeev formalism. Although this formalism is also applicable to the final atom-molecule state $|\mathcal{A}\Psi_f^{(-)}\rangle$, it is beyond the computational power of present supercomputers and we have to resort to an approximation. As a first step to a better understanding of the underlying reaction mechanism we formulated^{10,7} a model in which (in)elastic scattering was taken into account but rearrangement was excluded, selecting one pair to be bound throughout the scattering process and symmetrizing afterwards. Here we present a formulation which is symmetrical in all pairs from the start and hence leads automatically to the inclusion of rearrangement (the dipole-exchange mechanism). The subtle differences between these two approaches are made more explicit below.

Resonating-group theory¹⁴ is based on the variational principle

$$\langle \delta\psi | E - H | \psi \rangle = 0, \quad (5)$$

where $|\delta\psi\rangle$ and $|\psi\rangle$ are confined to a subspace of the total Hilbert space. The subspace to be used includes all possible open channels of atom-molecule scattering below the break-up threshold, with definite quantum numbers of total orbital angular momentum L and total electron spin angular momentum S to be specified shortly. This subspace is spanned by

$$\left\{ \begin{array}{l} |\mathcal{A}\Psi_f^{(-)}\rangle = \sum_{\alpha} |\psi_{\alpha}\rangle \\ |\psi_{\alpha}\rangle = \sum_{\nu\ell\lambda} \int dp p^2 \int dq q^2 \varphi_{\nu\ell}(p) \eta_{\nu\ell\lambda}(q) |pq(\ell\lambda)LM_L\rangle_{\alpha} |(s\frac{1}{2})SM_S\rangle_{\alpha} \end{array} \right. \quad (6)$$

using the usual Jacobi-coordinates and angular momentum basis in momentum space.¹³ In addition, $\varphi_{\nu\ell}(p)$ is the known singlet ($s=0$) bound state of pair α having the quantum numbers (ν, ℓ) and $\eta_{\nu\ell\lambda}(q)$ are unknown functions used in the variational principle (5) which describe the relative motion of atom α compared to the center of mass of the bound pair. We recall⁹ that in the zero temperature limit the final state $|\mathcal{A}\Psi_f^{(-)}\rangle$ has the quantum numbers $L=2$ and $S=\frac{1}{2}$, while $M_L=-1$ (-2) and $M_S=-\frac{1}{2}$ ($\frac{1}{2}$) in the case of a single (double) spin flip process. Furthermore, parity conservation requires $\ell+\lambda$ to be even. Because the total wavefunction is symmetric under permutations of the hydrogen atoms only odd ℓ values are allowed, $\eta_{\nu\ell\lambda}$ does not

depend on α and the vectors $|\psi_\alpha\rangle$ are related to each other by a cyclic permutation. It is important to point out that if we added to the bound states $\varphi_{v\ell}(p)$ the continuum of singlet scattering states $\varphi_{E\ell}(p)$ the complete Hilbert space would be spanned by Eq. (6) and the variational principle would give an exact solution of the three-body Schrödinger equation.

Performing the variation within the subspace defined above, we easily find the one-dimensional coupled integral equations for the functions $\eta_{v\ell\lambda}(q)$:

$$\eta_{v\ell\lambda}(q) = (1-(-1)^{\ell f}) \delta_{vv_f} \delta_{\ell\ell_f} \delta_{\lambda\lambda_f} \frac{\delta(q-q_f)}{qq_f} + \frac{1}{E - E_{v\ell} - 3q^2/4m_H} \sum_{v'\ell'\lambda'} \int dq' q'^2 v_{v\ell\lambda, v'\ell'\lambda'}(q, q') \eta_{v'\ell'\lambda'}(q') \quad (7)$$

where we made use of the linearity of the equations to simplify the inhomogeneous term.¹⁰ This term corresponds to the physical requirement that $|\mathcal{P}\psi_f^{(-)}\rangle$ contains asymptotically the plane waves $\mathcal{P}|\varphi_{v_f\ell_f m_f} \mathbf{q}_f\rangle_\alpha |(\mathcal{O}\frac{1}{2})\frac{1}{2}M_S\rangle_\alpha$ with the total energy $E = E_{v_f\ell_f} + 3q_f^2/4m_H$. Moreover, $E_{v\ell}$ is the energy of the bound state (v, ℓ) , m_H the hydrogen mass and the factor in front of the Kronecker deltas is a consequence of the statement made previously: Only odd values of the H_2 molecular angular momentum are allowed.

Introducing the operator $P = P_{12}P_{23} + P_{13}P_{23}$, i.e. the sum of the two cyclic permutation operators, we find for the "interaction" matrix of Eq. (7):

$$v_{v\ell\lambda, v'\ell'\lambda'}(q, q') = \int dp p^2 \varphi_{v\ell}(p) \int dp' p'^2 \varphi_{v'\ell'}(p') \times \alpha \langle pq(\ell\lambda)LM_L | \alpha \langle (\mathcal{O}\frac{1}{2})\frac{1}{2}M_S | \left\{ (1+P)V^\alpha - P(E-H_\alpha) \right\} | p'q'(\ell'\lambda')LM_L \rangle_\alpha | (\mathcal{O}\frac{1}{2})\frac{1}{2}M_S \rangle_\alpha \quad (8)$$

To see more clearly that rearrangement is indeed included, we consider the V^α and PV^α terms. The former gives rise to (in)elastic scattering without rearrangement. With only this term we recover the model of Ref. 10. In the context of the above-mentioned variational method this result is obtained if we asymmetrically restrict the subspace in which we solve the Schrödinger equation to all open channels (below break-up) of one particular pair α . In contrast, the term PV^α is responsible for the rearrangement process, since effectively a different particle pair is bound at either side of V^α . Finally, the contribution $-P(E-H_\alpha)$ accounts for the non-orthogonality of the vectors $|\psi_\alpha\rangle$. Intuitively, it guarantees that the Born series of Eq. (7) contains all possible interactions between the particles only once.

Formally Eq. (7) is identical to a two-body Lippmann-Schwinger equation and can be solved in the usual way by the introduction of the half-shell T(ransition)

matrix:

$$T_{v\ell\lambda, v_f\ell_f\lambda_f}(q, q_f, E) = \sum_{v', \ell', \lambda'} \int dq' q'^2 V_{v\ell\lambda, v'\ell'\lambda'}(q, q') \eta_{v', \ell', \lambda'}(q') . \quad (9)$$

To evaluate the "interaction" matrix numerically we rewrite $(1+P)V_\alpha$ as $V_\alpha P + PV_\alpha P$ and use the angular momentum representation of P .¹³ In the case of $PV_\alpha P$ this leads to a sum of triple integrals. Each of the triple integrals can be reduced to an integral over a product of two integrals if we use cubic splines¹⁵ to interpolate on the momentum arguments of the V_α -matrix. This procedure reduces the computational effort considerably but nevertheless the evaluation of the matrix elements of $PV_\alpha P$ is the most time-consuming part of our calculation.

III RESULTS AND DISCUSSION

A. Numerical results

We solved the model described in the previous section using Gauss-Legendre quadrature points to discretize the integral equation. To find converged results for the recombination rate constant L_g^{eff} we had to include all rotational levels with $v=12, 13, 14$ and in addition the (v, ℓ) states $(6-11, 1)$, $(8-11, 3)$ and $(11, 5)$. This leads to a total of 57 channels and a complex matrix equation for the half-shell T -matrix with a dimension of 1450. The inversion of this equation is performed by an LU-decomposition of the kernel. As mentioned above the main problem of the calculation is associated with the term $PV_\alpha P$ in the "interaction" matrix. Using the set of channels given, we had to sum over all angular momenta up to $\ell=9$ in the calculation of this term. Fortunately, it turns out that only $(13, 5)$, $(13, 7)$, $(14, 1)$ and most importantly $(14, 3)$ contribute significantly as final outgoing states to L_g^{eff} .

Before we present the results for the rate constant, we note that it is possible to extract immediately information on the collisional rovibrational relaxation of H_2 in the $1\Sigma_g^+$ electronic state, since we also evaluate the on-shell T -matrix. In Fig. 1 we summarize the branching ratios for the dominant elastic and inelastic relaxation processes from the $(14, 3)$ state downwards to the $v=12$ and 13 rotational levels in an $L=2$ collision. The probabilities depend of course on the relative momentum of atom and molecule and we have taken a value in agreement with the experimental situation at $E \approx 10T$, in which case the hydrogen molecules in the $(14, 3)$ state are formed in a recombination event with a kinetic energy of the order of 25K. From these results we conclude that on average the $(14, 3)$ molecule loses an energy of about 170K in the first collision with a b-atom in the gas. Note that in

our calculation only a total orbital angular momentum $L=2$ is used. In a more complete treatment of the collisional relaxation also angular momenta $L=3$ and 4 would have to be included. In view of this we do not give absolute cross-sections but only branching ratios, which should at least give an impression of orders of magnitude.

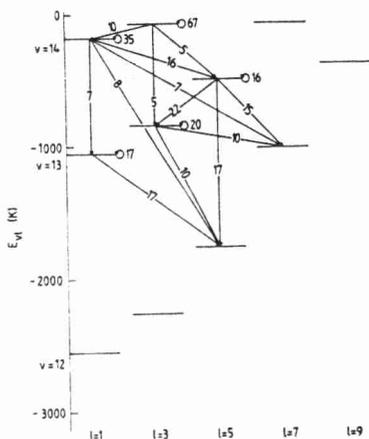


FIG. 1. The branching ratios (in %) for collisional rovibrational relaxation of highly excited H_2 molecules. Also indicated is the percentage for elastic collisions.

We now turn to the determination of L_g^{eff} . In Fig. 2 we give the three-body recombination rate constant as a function of applied magnetic field and compare both with experiment^{3,6} and our model without rearrangement.⁷ Neglecting for a moment the resonance structure, which we discuss more thoroughly in Sec. IIIB, we notice in general an almost magnetic field independent behavior of the background. Physically this can be understood as follows: Kagan's model⁸ predicted a steep increase of L_g^{eff} as a function of magnetic field, with a strong maximum around 15T. This behavior can be explained on the basis of the overlap in momentum space. The initial state contains three almost immobile atoms and in the final state the atom-molecule interaction is omitted. Since the magnetic dipole interaction induces only small momentum transfers, there is a strong preference for a slow final outgoing atom. On the other hand, phase-space arguments associated with the small q_f values explain the decrease of L_g^{eff} beyond 15T. Introducing an atom-molecule interaction in the rather weak form $\frac{3}{4}v^{(0)} + \frac{1}{4}v^{(1)}$, as we did in Refs. 7 and 10, shows already a tendency towards flattening. Although the repulsive $v^{(1)}$ and the attractive $v^{(0)}$ largely compensate one another in the relevant range of interatomic distances, the final state already contains such a range of momenta for any asymptotic q_f that the

preference for smaller q_f is reduced. Much higher momenta are coupled in when the full singlet or triplet interaction $V^{(s)}$ (depending on the parity of the relative angular momentum) is operating. We believe that this is the essential reason for the experimental behavior below 10T, most clearly displayed by the MIT data, which even show a slight decrease. It follows from the above arguments that any future extension of the approach of the present paper, including the full strength of $V^{(s)}$, will lead to the same qualitative feature of the L_g^{eff} curve.

For fields in the range 10-20T, we find a resonance-like behavior with maximum values far above the background. As we will describe in Sec. IIIB the explanation for this behavior is very different from the overlap arguments explaining Kagan's

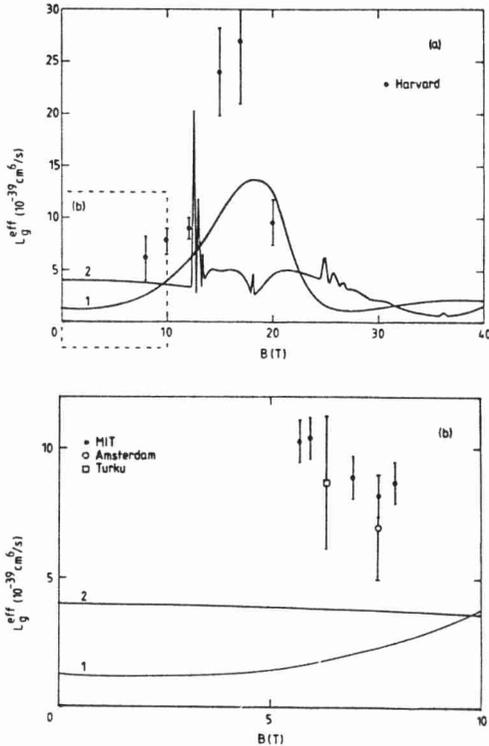


FIG. 2. The effective rate constant for three-body dipolar recombination of spin-polarized atomic hydrogen as a function of magnetic field. Figure (a) shows the range 0-40T, while figure (b) gives L_g^{eff} below 10T, in which range most of the experiments have been carried out. [Curve 1: The results of Refs. 10 and 7, without rearrangement. Curve 2: The results of the present calculation including rearrangement.] The experimental data is obtained from Refs. 3 and 6.

maximum. Although Kagan's model is in better agreement with the high-field data than our resonating-group approach (see Fig. 2(a) of Ref. 6), we stress that in our opinion it does not contain an essential ingredient. On the basis of the analysis of Sec. IIIB we believe that the recently measured high L_g^{eff} values can instead be explained by a bound-state calculation of the H_3 molecule, which is, however, outside the scope of the present paper.

Quantitatively, there is still strong disagreement. Below 10T our L_g^{eff} is a factor of two too small. In addition, the resonance peak at higher fields is too narrow and also does not have the correct position. As we show shortly this is due to an inadequate treatment of the resonances. To describe them correctly one needs to add singlet scattering states to the subspace defined by Eq. (6). However, due to divergences in the expressions for the "interaction" matrix it is not possible to do so directly. One possibility is to include some bounded wave packets into the variational principle. Since a wave packet is not an eigenstate of the channel Hamiltonian, this results in a much more complicated equation which does not have the structure of a two-body Lippman-Schwinger equation. In any case it is useful to have more information on the wavefunction of the resonance states. This will enhance physical insight into the reaction mechanism and may ultimately lead to an adequate description of the recombination process.

B. H_3 resonances

A convenient way to treat resonant scattering is by means of the Feshbach formalism.¹⁶ To do so we divide the total Hilbert space into two subspaces, conventionally denoted by P and Q, containing the open and closed channels of the scattering problem, respectively. Bound states in Q-space then correspond to resonances with finite lifetimes, because of the coupling between the two spaces.

In our case these subspaces can be characterized by the adiabatic states of three hydrogen atoms in an $1s^3 E'$ electronic configuration, having a total electron spin S equal to $\frac{1}{2}$. The potential surfaces are found by diagonalizing the 2×2 matrix

$$V_{SS}(\{r_\alpha\}) = \alpha \langle (s\frac{1}{2})SM_S | V | (s'\frac{1}{2})SM_S \rangle_\alpha,$$

which depends parametrically on the distances $\{r_\alpha\}$ between the particles.

Introducing the notation $V(r_\alpha) = \{V^{(1)}(r_\alpha) + V^{(0)}(r_\alpha)\}/2$ and $\Delta(r_\alpha) = V^{(1)}(r_\alpha) - V^{(0)}(r_\alpha)$ we easily find for the eigenvalues

$$V_{Q,P}(\{r_\alpha\}) = \sum_\alpha V(r_\alpha) \pm \frac{1}{2} \left\{ \sum_\alpha \Delta^2(r_\alpha) - \sum_{\alpha < \alpha'} \Delta(r_\alpha) \Delta(r_{\alpha'}) \right\}^{1/2}, \quad (10)$$

with Q(P) corresponding to the +(-) sign. If atom α' is far away from the other two

atoms, these energy surfaces reduce to the singlet and triplet potentials:

$$V_{Q,P}(\{r_\alpha\}) = V(r_{\alpha'}) \pm \frac{1}{2} \Delta(r_{\alpha'}) = V^{(1,0)}(r_{\alpha'}) .$$

leading to the conclusion that below break-up the open and closed channels of the atom-molecule collision can indeed be associated with the adiabatic states of the three-atom system.

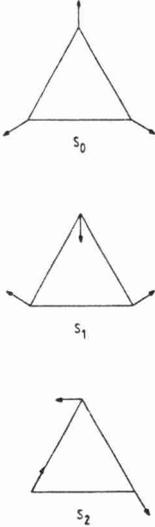


FIG. 3. The vibrational (external) symmetry coordinates S_i of an equilateral triangle.

We now concentrate on Q-space. For fixed $\sum_\alpha V(r_\alpha)$ the energy surface has a minimum if the atoms are in an equilateral configuration, because in that case the square root in Eq. (10) is zero. Therefore, one would like to introduce coordinates to describe the vibrations around this configuration. Since the depth of the Q potential surface is about 17000K and the calculations of the previous section show resonances with binding energies in the range of 35 to 50K, we are especially interested in highly excited states near the continuum ("long-range $H_{3\infty}$ molecules" 17). In this case the usual normal coordinates are not adequate. However, it is possible to introduce the (external) symmetry coordinates¹⁸ of an equilateral triangle having symmetry D_{3h} , which we denote by S_i ($i=1,2,3$).¹⁹ In Fig. 3 we see that S_0 corresponds to the symmetric-stretching mode, whereas S_1 and S_2 are two possible bending modes of the H_3 molecule.

The square root in Eq. (10) reducing to zero in the equilateral configuration, small deviations from this configuration, described by S_1 and S_2 , cause a steep linear¹⁹ increase in the potential energy. Physically, this means that the H_3

molecule carries out small-amplitude, rapid vibrations around an equilateral configuration that is vibrating more slowly with a large S_0 amplitude. In the following we, therefore, consider only potential terms up to first order in S_1 and S_2 but take all orders of S_0 into account.

The Hamiltonian of the rotating and vibrating non-linear molecule is given by^{18,20}

$$H = \frac{1}{2} (L-j)\mu(L-j) - \frac{\hbar^2}{8} \text{Tr}(\mu) - \frac{\hbar^2}{2m_H} \sum_i \frac{\partial^2}{\partial S_i^2} + V_Q(\{S_i\}) \quad (11)$$

where $L-j$ is the rotational angular momentum, j the vibrational angular momentum and μ the reciprocal inertia tensor, all defined with respect to an Eckart frame²¹ moving with the molecule. If we choose, in particular, the frame attached to the instantaneous orientation of the equilateral triangle we find that the vibrational angular momentum is perpendicular to the plane of the H_3 molecule and equal to

$$J_z = \left\{ S_2 \frac{\hbar}{i} \frac{\partial}{\partial S_1} - S_1 \frac{\hbar}{i} \frac{\partial}{\partial S_2} \right\} \quad (12)$$

Up to first order in S_1 and S_2 the tensor μ turns out to be

$$\mu = \frac{2}{m_H S_0^3} \begin{bmatrix} S_0 + 2S_1 & 2S_2 & 0 \\ 2S_2 & S_0 - 2S_1 & 0 \\ 0 & 0 & \frac{1}{2}S_0 \end{bmatrix} \quad (13)$$

Substituting these results into Eq. (11) and introducing polar coordinates (S_r, θ) instead of (S_1, S_2) we find the Hamiltonian

$$H = H^{\text{rot}} + H^{\text{vib}} + H^{\text{cor}} + V \quad (14)$$

with

$$H^{\text{rot}} + H^{\text{vib}} + V = \left\{ -\frac{\hbar^2}{2m_H} \frac{\partial^2}{\partial S_0^2} + \frac{\hbar^2}{2m_H S_0^2} [2L(L+1) - K^2 + 2KN + N^2 - \frac{5}{4}] + 3V(S_0) + \right. \\ \left. -\frac{\hbar^2}{2m_H} \frac{\partial^2}{\partial S_r^2} + \frac{\hbar^2}{2m_H S_r^2} [N^2 - \frac{1}{4}] + \beta(S_0)S_r \right\} \quad (15)$$

and H^{cor} a small perturbation due to the Coriolis force, which couples the rotation

and vibration of the molecule. Explicitly it reads

$$H^{\text{cor}} = \frac{S_r}{m_H S_0^3} \left\{ e^{i\vartheta} L_-^2 + e^{-i\vartheta} L_+^2 \right\}. \quad (16)$$

In the above expressions we have written the eigenvalues of L_z , and j_z , as $\hbar K$ and $-\hbar N$, respectively. Furthermore, in agreement with the approximations made, we have also expanded $V_Q(\{S_i\})$ up to first order in S_r leading to

$$V_Q(\{S_i\}) = 3V(S_0) + \left| \frac{3}{4} \frac{d\Delta(S_0)}{dS_0} \right| S_r \equiv 3V(S_0) + \beta(S_0) S_r,$$

which shows the above mentioned linear dependence of the potential surface on S_r .

Neglecting the Coriolis coupling for a moment we see that both K and N are good quantum numbers, because of the D_{3h} symmetry of the Hamiltonian of Eq. (15). The splitting of a particular vibrational level of the stretching mode, due to both the bending modes and the rotation of the H_3 molecule is shown qualitatively in Fig. 5(a), where the states with odd parity ($K=\pm 1$) are not considered, since they do not participate in the recombination process (cf. Sec. II). Also indicated is the degeneracy and the (D_3) symmetry class of the states.

Including H^{cor} breaks the D_{3h} symmetry down to D_3 and removes the degeneracy of the energy levels as is shown in Fig. 5(b). Only the levels corresponding to an E-type symmetry still have twofold degeneracy, which can be characterized by the conserved quantum number $2N-K$. Most importantly, we note that the spectrum of the (perturbed) $N=\pm 1$ states corresponds to the spectrum found in the calculation of Sec. IIIA, keeping in mind that the single and double spin-flip contributions to the rate constant cause the repetitive structure of $L_g^{\text{eff}}(B)$ at twice the magnetic field strength. From the numerically observed splitting between the two E-type levels we can estimate the average distance $\langle S_0 \rangle$ between the particles to be about $7a_0$. This

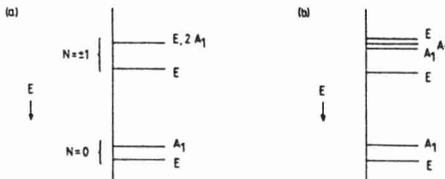


FIG. 4. The energy splitting of a vibrational level of H_3 stretching mode due to the bending modes and molecular rotation. (a) Without Coriolis coupling. (b) With Coriolis coupling.

gives the reason why the resonances are inadequately treated in our model: In the singlet bound states that span the subspace (6) the particles have on average a separation of at most $5a_0$, the (14,3) state having the largest dimensions. We thus have to include scattering states to make it possible for the particles to have larger separation. Extending the subspace in this manner we expect the resonances to be much broader, because the coupling with the P-space is enhanced, leading to a shorter resonance lifetime.

IV CONCLUSIONS

We have shown that in the three-body recombination process of spin-polarized atomic hydrogen, resonances play a crucial role and come into play when the possibility of rearrangement is included. In addition, we have identified these resonances with adiabatic states of an H_3 molecule in an almost equilateral configuration. Non-adiabatic effects, due to the finite kinetic energy of the atoms, lead to decay and therefore to a finite resonance lifetime. Our resonating-group method is able to explain the slow decrease of the recombination rate below 10T, as well as the occurrence of a much higher recombination rate at stronger fields. Despite this qualitative agreement with experiment, some features require a more thorough analysis which is at present out of reach: Below 10T our results are still a factor of two lower than experiment, while the resonance peaks at higher fields are too narrow and occur at too low a field value. This discrepancy requires a more adequate treatment of the H_3 resonance states, which are expected to have much wider interatomic separation than even in the case of a (14,3) H_2 molecule. Including singlet scattering states to allow for a large separation seems to be difficult in the context of the resonating group theory, since it involves non-localized wavefunctions. One possibility would be to use wavepackets instead.

Another approach, which has the advantage of using eigenstates of the channel Hamiltonian, was successfully applied to the triton²² and may also be used here. Since the three-body break-up channel is closed, the two-body continuum neglected in the ansatz (6) has to build up only a decaying state. Therefore, the channel Hamiltonian can be supplemented by an auxiliary confining potential conveniently chosen as a harmonic oscillator. This procedure leads to a discrete representation of the continuum and thus to a natural and rigorous extension of the calculations presented here.

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SUMMARY

This thesis deals with a central theme in sub-Kelvin physics: "cold" collisions and their role in experiments aiming at the achievement of Bose-Einstein condensation in spin-polarized atomic hydrogen gas. Some of the subjects studied pertain primarily to the more traditional high-density experimental scheme including its recent variants, others to low-density experiments involving magnetic traps and other advanced experimental techniques.

The thesis consists of seven chapters, which can be grouped in three parts. Chapter 1 is an introductory chapter giving the motivation and the general background of the thesis work. In addition, it places the Bogoliubov theory of a weakly interacting Bose gas, important for a more thorough understanding of Bose-Einstein condensation, in the context of QM_∞ . Finally, it justifies the elementary-boson picture of atomic hydrogen, which is used throughout the thesis.

Chapters 2, 3 and 4 are devoted to the determination of the decay constants for exchange and dipolar relaxation due to two-body collisions. Since two-body relaxation is the dominant decay mechanism of spin-polarized atomic hydrogen at relatively low densities this part of the thesis is particularly relevant to trapping schemes. We consider both the degenerate (Bose-Einstein condensed) and non-degenerate cases and also study the lifetime of an atomic hydrogen gas sample trapped in a microwave cavity. In the latter case we apply the very accurate degenerate-internal-states approximation, which is justified in Chapter 2 by means of rigorous coupled-channels calculations, to obtain reliable results without significant numerical effort.

In the last part (Chapters 5, 6 and 7) we turn to the theory of three-body scattering and more specifically to the evaluation of the rate constant for three-body dipolar recombination. In contrast with the two-body case rigorous calculations are very difficult and seem to lead beyond the (super)computing power available at present. Therefore, we have to resort to model calculations. Rather than reproducing experimental results quantitatively these are expected to reveal the reaction mechanism of the recombination process. To that end we arrive in Chapter 7 at our most sophisticated model, which we believe to contain all the essential physics. We find that resonances due to H_3 molecular states are of the utmost importance for the understanding of the recombination process. By means of them it is possible to explain recent experimental data qualitatively. Due to the approximate nature of the model significant discrepancies with experiment remain.

Further light on these discrepancies may be shed by an evaluation of the binding energy of rovibrational states of H_3 close to the continuum threshold. This seems numerically feasible and will be the subject of research in the near future.

SAMENVATTING

Dit proefschrift houdt zich bezig met een centraal thema in de lage-temperatuur fysica: "koude" botsingen en hun rol in experimenten gericht op het tot stand brengen van Bose-Einstein condensatie in spin-gepolariseerd atomair waterstof gas. Sommige van de behandelde onderwerpen zijn voornamelijk van toepassing op de traditionele experimenten bij hoge dichtheden met inbegrip van hun recente varianten, terwijl andere betrekking hebben op experimenten bij lage dichtheden waarbij gebruik gemaakt wordt van magnetische valkuilen en andere geavanceerde experimentele technieken.

Het proefschrift bestaat uit zeven hoofdstukken, die in drie groepen verdeeld kunnen worden. Hoofdstuk 1 is een inleidend hoofdstuk waarin de motivatie en de algemene achtergrond van het promotieonderzoek uiteen gezet wordt. Verder wordt de Bogoliubov theory van een zwak wisselwerkend Bose gas, die belangrijk is voor een beter begrip van Bose-Einstein condensatie, in de algemene context van QM_∞ geplaatst. Tenslotte geeft dit hoofdstuk een rechtvaardiging voor de in het gehele proefschrift gebruikte behandeling van atomair waterstof als een elementair deeltje met een boson karakter.

De hoofdstukken 2, 3 en 4 zijn gewijd aan de bepaling van de vervalsconstanten voor exchange- en dipolaire relaxatie ten gevolge van twee-deeltjes botsingen. Omdat twee-deeltjes relaxatie het belangrijkste vervalsproces is van spin-gepolariseerd atomair waterstof bij lage dichtheden, is dit gedeelte van het proefschrift in het bijzonder van belang voor experimenten met magnetische valkuilen. Wij besteden aandacht aan zowel het gedegeneerde (Bose-Einstein gecondenseerde) als het niet-gedegeneerde geval en bestuderen eveneens de levensduur van een hoeveelheid atomair waterstof gas gevangen in een microgolf trillholte. In het laatste geval maken we gebruik van de zeer nauwkeurige ontaarde-interne-toestanden benadering, die gerechtvaardigd wordt in hoofdstuk 2 met behulp van exacte gekoppelde kanalen berekeningen, om zonder veel numerieke inspanning betrouwbare resultaten te verkrijgen.

In het laatste gedeelte (de hoofdstukken 5, 6 en 7) richten wij ons op de theorie van drie-deeltjes verstrooiing en meer in het bijzonder op de bepaling van de vervalsconstante voor drie-deeltjes dipolaire recombinitie. In tegenstelling tot

het geval van twee deeltjes zijn exacte berekeningen zeer moeilijk en van een omvang die uitstijgt boven de mogelijkheden van hedendaagse (super)computers. Daarom moeten wij ons beperken tot model berekeningen, waarvan niet verwacht kan worden dat ze experimentele resultaten quantitatief reproduceren maar wel dat ze informatie opleveren over het reactie mechanisme van het recombinitie proces. Met dit doel voor ogen presenteren wij in hoofdstuk 7 ons meest geavanceerde model, waarvan wij geloven dat alle essentiële fysica erin vervat is. Hieruit blijkt dat resonanties als gevolg van rovibrationele toestanden van het H_3 molecuul van het grootste belang zijn voor een begrip van het recombinitie proces. Met behulp hiervan is het mogelijk experimentele gegevens kwalitatief te verklaren. Vanwege het benaderende karakter van het model blijven er echter significante afwijkingen met het experiment bestaan. Er zou meer licht op deze discrepanties geworpen kunnen worden door een bepaling van de bindingsenergie van de rovibrationele toestanden van H_3 dicht bij de continuüm drempel. Dit lijkt numeriek haalbaar en zal het onderwerp zijn van verder onderzoek in de nabije toekomst.

STELLINGEN

behorende bij het proefschrift van

H.T.C. Stoof

1. Volgens een algemeen verbreide opvatting, onder meer verwoord door Snoke en Wolfe, kan in een gas een macroscopische bevolking van de een-deeltjes grondtoestand in een eindige tijd tot stand komen door drie-deeltjes botsingen. Deze opvatting is onjuist.

D.W. Snoke en J.P. Wolfe, Phys. Rev. B39, 4030 (1989)

2. Analooq aan de behandeling van de voortplanting van radiogolven rond de aarde door Sommerfeld kan het microgolfveld in een concentrische Fabry-Perot interferometer op een elegante manier bepaald worden door gebruik te maken van complexe waarden van het impulsmoment quantumgetal ℓ .

A. Sommerfeld, Vorlesungen über theoretische Physik, Band VI (Dieterich'sche Verlagsbuchhandlung, Wiesbaden, 1947)

3. Ten gevolge van het optreden van Bose-Einstein condensatie neemt de reactieconstante van een N-deeltjes proces bij het absolute nulpunt af met een factor $N!$.

H.T.C. Stoof, A.M.L. Janssen, J.M.V.A. Koelman en B.J. Verhaar, Phys. Rev. B39, 3157 (1989)

4. Voor het toepasbaar zijn van de door Lee en Yang ontwikkelde theorie van een zwak wisselwerkend Bose gas moeten niet alleen de parameters $(na^3)^{\frac{1}{2}}$ en na^2 zelf, maar tevens hun verhouding $(na^3)^{\frac{1}{2}}/na^2$ klein zijn.

T.D. Lee en C.N. Yang, Phys. Rev. 112, 1419 (1958);

H.T.C. Stoof, A.M.L. Janssen, J.M.V.A. Koelman en B.J. Verhaar, Phys. Rev. B39, 3157 (1989)

5. De eerste-orde faseovergang die optreedt in inflatiemodellen voor het ontstaan van het universum is equivalent met Bose-Einstein condensatie van het Higgs veld.
6. In de terminologie van de quantum optica is de grondtoestand van een zwak wisselwerkend Bose gas een 'squeezed vacuum'.

7. De reflectie van waterstof atomen aan een superfluïde heliumfilm is in zeer goede benadering onafhankelijk van de adsorptie potentiaal.
8. Het gebruik van een gelijkheid als $|\alpha\rangle = \psi_\alpha(\vec{r})$ in sommige fysische publicaties getuigt van onvoldoende inzicht in het verschil tussen een toestandsvector en zijn representatie.

W.A. Harrison, *Pseudopotentials in the theory of metals* (W.A. Benjamin Inc., New York, 1966)

9. De door Umberto Eco gegeven verklaring voor het gedrag van de slinger van Foucault is literair gezien wellicht verantwoord maar fysisch onjuist.

U. Eco, *De Slinger van Foucault* (Bert Bakker, Amsterdam, 1989)

10. Ter voorkoming van onnodige dubbelzinnigheden zou het in de Japanse taal gebruikte logisch juiste antwoord op ontkennende vragen ook in de Nederlandse spreektaal ingevoerd moeten worden.