

# Collisional two- and three-body decay rates of dilute quantum gases at ultralow temperatures

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In view of recent successful evaporative cooling experiments reaching temperatures in the nK range, we discuss ground-state two-body inelastic and three-body decay rates of dilute cold atomic gas samples at ultralow temperatures. We present theoretical low-temperature two-body decay rates in alkali-atom systems using recently obtained information on two-body potentials. The rates show an oscillating structure as a function of temperature and magnetic field which can be understood in terms of the interference of initial and final radial waves.

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The recent breakthrough [1] in the ongoing attempts to realize the Bose-Einstein condensed phase in a dilute quantum gas by evaporative cooling (see also Refs. [2–4]) makes it increasingly important to predict the rates of the two-body inelastic and three-body collisional decay mechanisms of the gas density in the  $T \rightarrow 0$  temperature limit, since these are expected to control primarily the lifetime of the condensate. Some recent work addresses this question [5,6]. In this paper we present some results for two-body inelastic collisional rates for  $T \rightarrow 0$ , calculated by a rigorous quantum-mechanical approach and using recently obtained information on two-body potentials. A discussion is also devoted to three-body decay in this limit.

Let us first discuss the inelastic decay rate due to two-body exchange collisions. As an example we consider the transitions

$$(1, -1) + (2, +1) \rightarrow (1, -1) + (1, +1) \\ \rightarrow (1, 0) + (1, 0) \quad (1)$$

due to exchange collisions in either  $^7\text{Li}$ ,  $^{23}\text{Na}$ , or  $^{87}\text{Rb}$ , using the notation  $(f, m_f)$  for single-atom hyperfine states. The processes (1) may be of importance as a loss mechanism in gravitational Sisyphus cooling [7,8]: they are exothermal and, moreover, the final  $(1, 0)$  and  $(1, +1)$  states are high-field seeking. Figure 1 shows the energy dependence of the rate constants of processes (1) before thermal averaging at zero magnetic field, calculated by means of the quantum-mechanical coupled-channels method using the triplet and singlet Na-Na potentials of Refs. [9,10]. Note that the rates go to a finite limit for the collision energy  $E$  in the entrance channel going to 0. This is in agreement with Wigner's threshold law [11]. Previously, (finite) values for the same  $T=0$  relaxation rates were obtained by our group in the case of spin-polarized hydrogen [12,13]. If one would apply the semiclassical approximation, expected to be valid at higher energy [14], to describe the radial motion at ultralow collision energies in the initial channel, one would obtain a rate going to infinity as  $E^{-1/2}$  (see also Fig. 3 below). This is also the conclusion of Ref. [5]. Note that the quantum suppression effect indicated in that paper is a relative suppression of the rigorous quantum rates compared to semiclassical values. It is not an absolute suppression in the sense that quantum

rates go to zero for  $T \rightarrow 0$ . In this connection it is of interest to point to an important difference of three-dimensional (3D) quantum reflection with that of ultracold atoms against a superfluid helium film, which is essentially a 1D scattering phenomenon. Although the  $s$ -wave radial Schrödinger equation in 3D has the same fundamental form as the 1D Schrödinger equation, the quantum reflection phenomenon is different in 3D and 1D. This can be illustrated most easily by comparing the scattering of a wave with a long wavelength and an amplitude of 1 by a hard object in 1D and 3D. In 1D the destructive interference of the reflected wave with the incoming one strongly reduces the total wave amplitude with respect to 1 within a distance of the order of the wavelength. In 3D the scattered wave spreads out isotropically, so that the strong destructive interference extends only over a small fraction of a wavelength. Quantitatively this follows for general potentials from the expression  $(1/kr)\text{sinc}(r-a)$  for the total wave function in the region just outside the scatterer, which goes to the finite value  $1-a/r$  for  $k \rightarrow 0$ , whereas the total wave in 1D will behave like  $\text{sinc}(z-a)$ , going to zero as  $k(z-a)$ .

Next we turn to the process of relaxation of the doubly polarized atomic states due to the magnetic dipolar spin-spin interaction. The rate constant for this process is given by

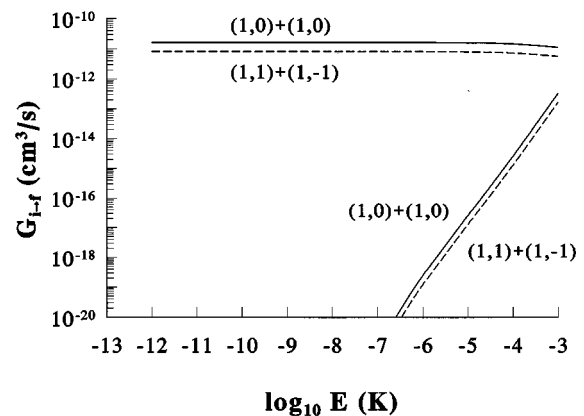


FIG. 1. Exchange  $s$ -wave (upper curves) and  $d$ -wave (lower curves) relaxation rates  $G_{i \rightarrow f}$  for the processes  $(2, +1) + (1, -1) \rightarrow (1, +1) + (1, -1)$  and  $(2, +1) + (1, -1) \rightarrow (1, 0) + (1, 0)$  in Na as a function of energy in the initial channel.

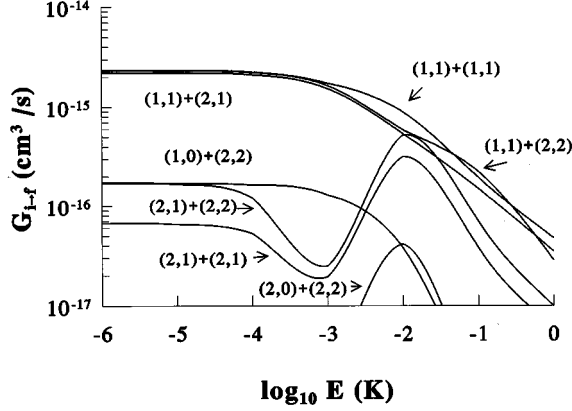


FIG. 2. Dipolar relaxation rates  $G_{i \rightarrow f}$  for the doubly polarized  $(2, +2)$  Na gas for  $B = 1$  mT as a function of energy. The symbols  $(f_1, m_{f_1}) + (f_2, m_{f_2})$  denote the final collision channel.

$$G_{i \rightarrow f} = \frac{\pi m k_f}{(2\pi\hbar)^3} \int d\hat{k}_f |T_{fi}(\vec{k}_f, \vec{k}_i)|^2, \quad (2)$$

with  $\vec{k}_i$  and  $\vec{k}_f$  the initial and final wave vectors. In Eq. (2) the normalization of the  $T$ -matrix element is taken to be such that its lowest-order form in terms of the interatomic interaction is

$$T_{fi}^0(\vec{k}_f, \vec{k}_i) = \int (e^{i\vec{k}_f \cdot \vec{r}})^* V e^{i\vec{k}_i \cdot \vec{r}} d^3r. \quad (3)$$

Treating the weak dipolar interaction  $V^d$  to first order and the central (singlet-triplet) potential to infinite order, we have

$$T_{fi}(\vec{k}_f, \vec{k}_i) = \int u_f^*(\vec{k}_f, \vec{r}) V^d u_i(\vec{k}_i, \vec{r}) d^3r, \quad (4)$$

where  $u_i$  and  $u_f$  are distorted waves. In Eqs. (3) and (4) we have suppressed the spin degrees of freedom in the notation. Now consider as an example the transition

$$(2, +2) + (2, +2) \rightarrow (2, +2) + (2, +1) \quad (5)$$

at a field  $B \neq 0$ . In this case both  $u_i$  and  $u_f$  are pure triplet waves with  $l_i = 0$  and  $l_f = 2$ . For small  $k_i$ ,  $k_f$  remains finite and  $u_i(\vec{k}_i, \vec{r})$  goes to an isotropic function in the radial range where the dipolar transition takes place and is given by the above function  $(1/kr)\text{sink}(r-a) \approx 1-a/r$ . As a consequence,  $T_{fi}$  and  $G_{i \rightarrow f}$  go to a finite constant, again in agreement with Wigner's threshold law [11] and Ref. [5].

The rate of the process (5) for Na is presented in Fig. 2, together with those of all other possible final channels. At higher collision energies  $d$ -wave and higher partial-wave contributions would have to be added as in Fig. 1, but we leave them out since they are not relevant for the ultralow temperatures under consideration. The oscillating behavior that is seen in Fig. 2 for some of the final channels is analogous to that for atomic hydrogen [15,16] and is most easily understood by approximating the distorted waves by plane waves,

$$T_{fi}(\vec{k}_f, \vec{k}_i) \sim r_{20} = \int j_2(k_f r) \frac{1}{r} j_0(k_i r) dr, \quad (6)$$

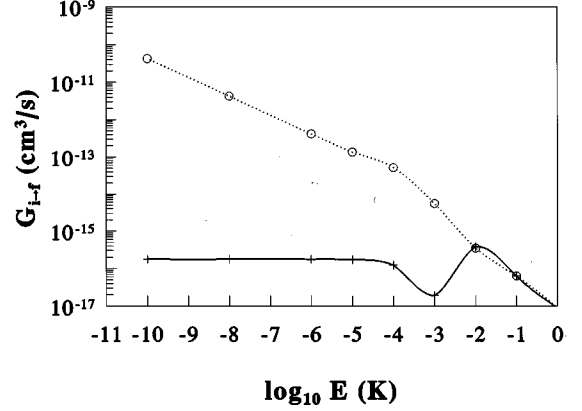


FIG. 3. Dipolar relaxation rate  $G_{(2, +2) + (2, +2) \rightarrow (2, +1) + (2, +2)}$  for  $B = 1$  mT calculated with semiclassical approximation (dashed line) and with a quantum-mechanical calculation (solid line).

and expanding the radial integral in powers of  $k_i/k_f$  [15]:

$$r_{20} = \frac{1}{3} \left( 1 - \frac{k_i^2}{k_f^2} + \dots \right), \quad (7)$$

which leads to

$$G_{i \rightarrow f}(B, T) \sim \sqrt{\Delta\epsilon(B)} \left[ 1 - \frac{9k_B T}{4\Delta\epsilon(B)} + \dots \right]. \quad (8)$$

In Fig. 3 we compare the quantum-mechanical dipolar rate of Fig. 2 for the specific process (5) with that in the semiclassical approximation, i.e., using radial WKB wave functions. Clearly, at ultralow energies the semiclassical rate goes to infinity as  $E^{-1/2}$ , overestimating the quantum rate by more than two orders of magnitude at 1 mK and more than three at 1  $\mu$ K.

In Fig. 4 the relaxation rates for zero temperature as a function of magnetic field are shown, calculated by the full coupled-channels method. In agreement with (2) processes for which the exothermal energy  $\Delta\epsilon(B)$  goes to 0 for  $B \rightarrow 0$  have a negligible phase-space available for decay, so that their rate goes to 0 [see, also, Eq. (2)]. The oscillations in some of the channels are again due to the interference of initial and final radial wave functions, as described previously in Eq. (6). The exact  $B$ -field locations of the oscillations in the coupled-channel results can be reproduced by taking triplet distorted waves in the radial integral  $r_{20}$ , i.e., the oscillations depend on the specific properties of the triplet potential. In Fig. 5 we give the same field-dependent dipolar rates for  $^7\text{Li}$ . A comparison of the present rates for Na, calculated with the recently obtained potentials and accumulated radial phase [9,10], with results in an earlier publication [17] shows that the dominant rates differ by less than one order of magnitude. Understandably, the weaker transitions are more sensitive to potentials.

We now turn to three-body recombination. The possibility that the rate for this process might show a suppression phenomenon, as a consequence of which it would vanish for  $T \rightarrow 0$ , has been considered recently [6]. This result would be inconsistent with the results of the work in our group on spin-polarized atomic hydrogen several years ago [18], in

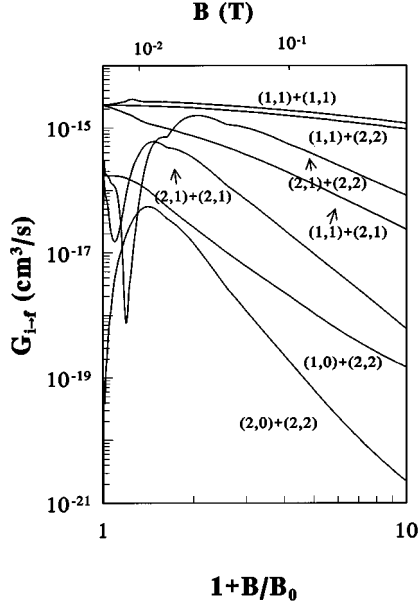


FIG. 4. Zero-temperature dipolar relaxation rates  $G_{i \rightarrow f}$  for the doubly polarized (2,+2) Na gas as a function of magnetic field. Horizontally the quantity  $1+B/B_0$  with  $B_0 = a/\hbar \gamma_e = 0.0316$  T is plotted logarithmically. The symbols  $(f_1, m_{f_1}) + (f_2, m_{f_2})$  denote the final collision channel.

which the zero-energy limit of the three-body collisional wave function was calculated for three doubly spin-polarized hydrogen atoms by solving the Faddeev equations rigorously for  $E=0$ . The resulting wave function has finite values for the three atoms at relative distances, where it should vanish according to the prediction of Ref. [6]. To discuss the low-energy limit let us take the rate constant expression for three-body dipolar recombination [18],

$$L_{i \rightarrow f} = \frac{\pi m k_f}{6(2\pi\hbar)^3} \int d\vec{k}_f |T_{fi}(v l m \vec{k}_f, \vec{k}_i \vec{K}_i)|^2, \quad (9)$$

analogous to Eq. (2) with  $v l m$  the quantum numbers of the final diatom rovibrational state,  $\vec{k}_f$  the final relative atom-diatom wave vector, and  $\vec{k}_i, \vec{K}_i$  the initial Jacobi wave vectors. To first order in  $V^d$ ,  $T_{fi}$  is given by an integral,

$$T_{fi} = \int u_f^*(v l m \vec{k}_f, \vec{\rho}) V^d u_i(\vec{k}, \vec{\rho}) d^6 \rho \quad (10)$$

in 6D configuration space. The plane-wave parts of the  $u_i$  and  $u_f$  functions are normalized as exponential plane waves. In particular, as  $e^{i\vec{k} \cdot \vec{\rho}}$  for  $u_i$  with  $\vec{k}$  the 6D initial wave vector. Reference [6] points out that the suppression of the initial wave would take place already in the free case because of the

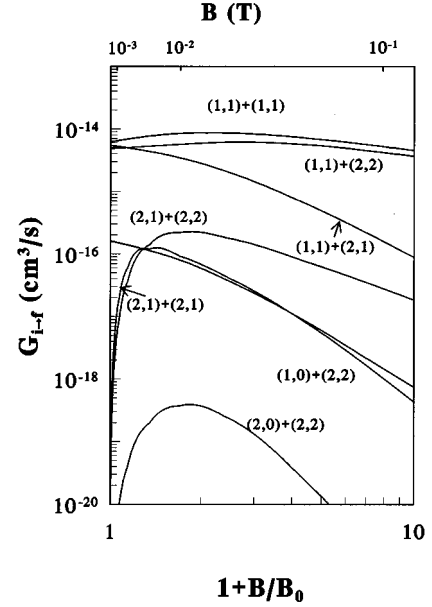


FIG. 5. Zero-temperature dipolar relaxation rates  $G_{i \rightarrow f}$  for the doubly polarized (2,+2)  $^7\text{Li}$  gas as a function of magnetic field. Horizontally the quantity  $1+B/B_0$  with  $B_0 = a/\hbar \gamma_e = 0.0143$  T is plotted logarithmically. The symbols  $(f_1, m_{f_1}) + (f_2, m_{f_2})$  denote the final collision channel.

positive 6D centrifugal term  $15/8 \mu \rho^2$  occurring in the 6D radial wave equation for the lowest hyperspherical partial wave. It should be noted, however, that in the low-energy approximation the free wave  $u_i^0$  is again isotropic and equal to  $8J_2(\kappa\rho)/(\kappa\rho)^2$  (see also the plane-wave expansion in any dimension in hyperspherical coordinates in Ref. [19]). For  $\kappa \rightarrow 0$  this function tends to 1 as it should. However, the solution of the 6D radial wave equation, which is normalized as a sine function at infinity, is equal to  $J_2(\kappa\rho)(\kappa\rho/2)^{1/2}$ , and this indeed tends to 0 in the limit  $\kappa \rightarrow 0$  for fixed finite  $\rho$ .

In summary, we have presented predictions for low-temperature two-body decay rates in alkali-atom systems using recently obtained information on two-body elastic collision properties. The dipolar decay rates show an oscillating structure as a function of temperature and magnetic field, which find their origin in the relative displacements of the oscillation patterns in the  $l_i=0$  initial and  $l_f=2$  final radial wave functions with varying  $k_f$  (or  $k_i$  and  $k_f$ ). Finally we also discussed the behavior of the three-body recombination rate in the zero-energy limit.

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