Internal State Conversion in Ultracold Gases

J. N. Fuchs,* D. M. Gangardt,[†,‡] and F. Laloë[§]

LKB, Laboratoire de Physique de l'ENS, 24 rue Lhomond, 75005 Paris, France

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We consider an ultracold gas of (noncondensed) bosons or fermions with two internal states, and we study the effect of a gradient of the transition frequency between these states. When a $\pi/2$ rf pulse is applied to the sample, exchange effects during collisions transfer the atoms into internal states which depend on the direction of their velocity. This results, after a short time, in a spatial separation between the two states. A kinetic equation is solved analytically and numerically; the results agree well with the recent observations of Lewandowski *et al.*

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In the last few years, the study of ultracold gases has generated a wealth of very interesting results. Spectacular examples are given by Bose condensed gases, but gases above their degeneracy temperature also provide exciting and unexpected results. For instance, recent experiments by Lewandowski *et al.* [1] have shown the existence of a remarkable phenomenon, observed when a rf pulse is applied to a ^{87}Rb gas with two internal states, cooled by laser irradiation and evaporative cooling (but not Bose condensed). Since the two internal states are similar to two different species of atoms, the authors describe their observation as a "segregation" between the species. They also mention that the differential Stern-Gerlach force, due to the magnetic gradient acting on the species, is too small to explain the segregation, which is actually related to interactions between the atoms. The purpose of the present Letter is to show that the "identical spin rotation effect" (ISRE) provides a qualitative and a quantitative explanation of the observations.

The ISRE was introduced in [2] as a microscopic phenomenon taking place during a binary collision between two identical atoms with internal degrees of freedom, nuclear spins, for instance. The effect is a consequence of quantum indistinguishability; it introduces a rotation of each spin around their sum (in opposite directions for bosons and fermions). For instance, if a single atom with a spin polarization in a given direction crosses a gas of identical atoms polarized in another direction, the spin of the transmitted atom undergoes a rotation; this is similar to the rotation of the polarization of photons in the Faraday effect. On a macroscopic scale, the effect can affect transport properties of gases with internal states. For instance, Ref. [3] considers a gas which is in a "classical" regime in terms of equilibrium properties, but where quantum effects are important in binary collisions. When the density is sufficient to reach a hydrodynamic regime, this work shows the existence of transverse spin waves, analogous to spin waves in degenerate liquid ^{3}He [4]. Similar predictions had been made independently by Bashkin [5] from a more macroscopic point of view, based on the notion of "molecular field" (or mean field)—see also the work of Lévy and Ruckenstein [6]. Transverse spin waves in gases were subsequently observed in H↓ [7] as well as in helium [8,9].

Another prediction made in Ref. [3] (end of Sec. 1) is that the ISRE can also create "longitudinal oscillations" when a $\pi/2$ pulse is applied to the sample, provided the transverse spin polarization is inhomogeneous. Here we show that the phenomenon described in Ref. [1] is precisely this effect, transposed to the pseudospin associated with the two hyperfine levels relevant in the experiment, as foreseen by the authors who mention a "longitudinal spin effect" in their conclusion. The major differences are that the experiment was performed at a density where the hydrodynamic regime is not reached and that the spin oscillations are not of small amplitude.

A point which emerged from the early studies on spin waves in gases, sometimes after vivid controversy, is that the effect of binary collisions in a gas are well described by a simple mean field calculation, provided one considers forward scattering only. In condensed matter, each particle interacts at the same time with several others; it seems natural that their individual effects should be well averaged by the test particle so that mean field theory should apply. By contrast, in a dilute gas, particles are "free almost all the time"; they interact only during brief collisions, with a single partner with which they can develop strong correlations. Indeed, in atomic physics, one rarely studies collision processes within mean field theory. Nevertheless, it turns out that the average effect of many collisions in the forward direction is equivalent to the results of mean field theory, if one replaces the real binary interaction potential by a pseudopotential involving directly the scattering length (using the real potential would lead to meaningless results); the equivalence holds in the limit of low collision energy (the ISRE in the forward direction dominates over lateral scattering at very low energies since the corresponding "cross section" $\tau_{\mathrm{ex}}^{\mathrm{fwd}}$ diverges [2]).

In the experimental conditions of Ref. [1], the atoms are in an axially symmetric magnetic trap elongated in the Ox direction. Initially the gas is at equilibrium with only state 1 populated. One then applies a $\pi/2$ rf pulse which, suddenly, puts all the atoms into the same coherent superposition of states 1 and 2, corresponding to a uniform

transverse polarization of the pseudospin. The system is then left free to evolve, and one observes the time evolution of the local densities n_1 and n_2.

We begin with a qualitative physical discussion of the sequence of events. Since the field gradient creates an inhomogeneous spin precession, the gas develops a gradient of transverse spin orientation: correlations are created between position and transverse spin orientation. The free thermal motion of the atoms then creates correlations between velocity and transverse spin. Thus, a particle moving with a given velocity at point x gets a spin polarization which is not parallel to the average local spin polarization, so that the ISRE precession takes place. This makes its spin polarization leave the transverse plane and develop a nonzero value of its longitudinal component, with an opposite sign for different signs of the x component of the velocity of the atom. The appearance of this component indicates the beginning of an internal conversion, which eventually results in spatial separation of the atoms in different internal states. We emphasize that the apparent segregation is not the result of a spatial separation of atoms in fixed internal states, as for two different chemical species; on the contrary, without changing their spatial position, the ISRE transfers atoms into internal states that depend on their motion.

For a more quantitative discussion, we use a transport equation in terms of a time t dependent operator $\hat{\rho}(\mathbf{r}, \mathbf{p}, t)$, which depends on position $\mathbf{r}$ and momentum $\mathbf{p}$; $\hat{\rho}$ is the Wigner transform with respect to orbital variables of the single particle density matrix; it remains a 2×2 operator in the space of internal variables, corresponding to states 1 and 2. Instead of using the four matrix elements of $\hat{\rho}$, it is often convenient to replace them by a local density f and (pseudo) spin density $\mathbf{M}$ in phase space defined by

$$\hat{\rho}(\mathbf{r}, \mathbf{p}, t) = \tfrac{1}{2}[f(\mathbf{r}, \mathbf{p}, t)\hat{I} + \mathbf{M}(\mathbf{r}, \mathbf{p}, t) \cdot \hat{\sigma}], \quad (1)$$

where $\hat{I}$ is the unit operator in spin space and $\hat{\sigma}$ is the spin operator whose three components are the Pauli matrices. The kinetic equation for $\hat{\rho}(\mathbf{r}, \mathbf{p}, t)$ (see, for instance, [2]) is

$$\partial_t \hat{\rho} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} \hat{\rho} - \frac{1}{2}[\nabla_{\mathbf{p}} \hat{\rho}, \cdot \nabla_{\mathbf{r}} \hat{U}(\mathbf{r}, t)]_+ + \frac{1}{i\hbar}[\hat{\rho}, \hat{U}(\mathbf{r}, t)]_- = I_{\mathrm{coll}}[\hat{\rho}], \quad (2)$$

where the second term is the usual drift term (m is the mass of the particles); the third term (anticommutator) is the force term including both the effect of the trapping potential and of the mean field created by the other atoms; the fourth term (commutator) is a spin precession term containing the ISRE as well as some other contributions that we discuss below—this commutator is the term on which we focus our attention in this Letter. On the right-hand side, the collision integral $I_{\mathrm{coll}}[\hat{\rho}]$ describes "real" collisions (lateral scattering as opposed to forward scattering, already included in the mean field); it can be obtained, for instance, from the Lhuillier-Laloë transport equation [2], or even take a more detailed expression containing "nonlocal collision terms" with $\mathbf{r}$ and $\mathbf{p}$ gradients, as discussed, e.g., in the appendix of [10] and [11]. In fact, if we are mostly interested in a Knudsen regime, the precise expression of $I_{\mathrm{coll}}[\hat{\rho}]$ is not needed. The effective potential $\hat{U}(\mathbf{r}, t)$ is the spin operator

$$\hat{U}(\mathbf{r}, t) = U_0(\mathbf{r}, t)\hat{I} + \mathbf{U}(\mathbf{r}, t) \cdot \hat{\sigma}, \quad (3)$$

where the scalar component is defined by

$$U_0 = \frac{V_1 + V_2}{2} + g^{\epsilon}_{22} n_2 + g^{\epsilon}_{11} n_1 + \frac{g^{\epsilon}_{12}}{2}(n_2 + n_1). \quad (4)$$

Here V_1 and V_2 are the external trapping potentials acting on states 1 and 2; the g^{ϵ}'s have the following expressions in terms of the usual "coupling constants" g, proportional to the appropriate scattering lengths associated with the various possibilities for pair interactions between atoms in levels 1 or 2 [12]:

$$g^{\epsilon}_{11,22} = g_{11,22}(1 + \epsilon)/2; \qquad g^{\epsilon}_{12} = g_d + \epsilon g_t, \quad (5)$$

where g_d and g_t refer to the direct and transfer process for two atoms in different levels. The number densities of atoms in levels 1 and 2 are $n_{1,2}$; $\epsilon = +1$ (-1) for bosons (fermions). The vectorial component of $\hat{U}(\mathbf{r}, t)$ is

$$\mathbf{U}(\mathbf{r}, t) = \frac{\hbar\Omega(\mathbf{r}, t)}{2}\mathbf{e}_{\parallel} + \epsilon \frac{g^{\epsilon}_{12}}{2}\mathbf{m}(\mathbf{r}, t); \quad (6)$$

$\mathbf{e}_{\parallel}$ is the unit vector in the longitudinal spin direction, and $\Omega(\mathbf{r}, t)$ is

$$\hbar\Omega = V_2 - V_1 + 2g^{\epsilon}_{22} n_2 - 2g^{\epsilon}_{11} n_1 + 2g^{\epsilon}_{12}(n_1 - n_2), \quad (7)$$

where the total density n and spin polarization $\mathbf{m}$ are

$$n(\mathbf{r}, t) = \int d^3p\, f(\mathbf{r}, \mathbf{p}, t); \qquad \mathbf{m}(\mathbf{r}, t) = \int d^3p\, \mathbf{M}(\mathbf{r}, \mathbf{p}, t) \quad (8)$$

and $n_{1,2} = (n \mp m_{\parallel})/2$. The first contribution (7) to $\mathbf{U}$ acts as a "local magnetic field"; its average value over the sample can be removed in a uniformly rotating frame. The second contribution originates from the ISRE and is proportional to the local spin polarization $\mathbf{m}$ (only $\mathbf{m}$ enters the ISRE commutator because the $1/k$ divergence of $\tau^{\mathrm{fwd}}_{\mathrm{ex}}$ at low k's [2] compensates the relative velocity factor of the collision integral). The commutator makes $\mathbf{M}$ precess around the momentum integrated local spin polarization; it does not affect the evolution of $\mathbf{m}$ itself but can change the evolution of $\mathbf{M}$ for each value of $\mathbf{p}$.

A few simplifying assumptions are appropriate in the experimental conditions of [1]. The confining energy is of order $k_B T \simeq 13$ kHz $\times h$ which is much larger than the mean field interaction energy $gn(0) \simeq 140$ Hz $\times h$ and

the differential trapping energy $V_1 - V_2 \sim 10\ \mathrm{Hz} \times h$. In the anticommutator this allows us to retain only the confining energy of the harmonic trap:

$$U_0 \simeq \frac{V_1 + V_2}{2} = \frac{1}{2} m[\omega^2 x^2 + \omega_{\mathrm{rad}}^2 (y^2 + z^2)]; \quad (9)$$

here ω and ω_{rad} are the axial and radial trapping frequencies. In the commutator of (2), U_0 disappears, and only the vectorial component $\mathbf{U}$ plays a role. The cigar shaped trap has an axial frequency $\omega/2\pi = 7$ Hz, much smaller than the radial frequency $\omega_{\mathrm{rad}}/2\pi = 230$ Hz, so that the system is quasi-one-dimensional along the x axis. Assuming that radial local equilibrium is quickly established in the yz plane, we introduce the on-axis value $\hat{\rho}(x, p, t)$ (integrated over radial momenta). When averaged over radial coordinates and momenta, Eq. (6) becomes

$$\overline{\mathbf{U}}(x, t) = \hbar \overline{\Omega}(x) \mathbf{e}_{\parallel}/2 + \epsilon g_{12}^{\epsilon} \mathbf{m}(x, t)/4, \quad (10)$$

where $\hbar\overline{\Omega} = \overline{V}_2 - \overline{V}_1 + (g_{22}^{\epsilon} - g_{11}^{\epsilon})n/2$; note that the coupling constants are renormalized by a factor of $1/2$ upon averaging [13]; we have assumed that $2g_{12}^{\epsilon} \simeq g_{11}^{\epsilon} + g_{22}^{\epsilon}$.

With these assumptions the initial equilibrium Maxwell-Boltzmann distribution $f(x, p)$ solves the kinetic equation (2), so that the dynamics after the pulse can be expressed in terms of $\mathbf{M}$ only. When lengths are measured in units of $x_T = \sqrt{k_B T/m\omega^2}$, momenta in units of $p_T = \sqrt{m k_B T}$, and times in units of $1/\omega$, Eq. (2) simplifies into

$$\partial_t \mathbf{M} + p\partial_x \mathbf{M} - x\partial_p \mathbf{M} - \frac{2\overline{\mathbf{U}}}{\hbar\omega} \times \mathbf{M} \simeq -\frac{\mathbf{M} - \mathbf{M}^{\mathrm{eq}}}{\omega\tau_M}, \quad (11)$$

where a simple relaxation-time approximation has been made for I_{coll} with a single parameter τ_M of the order of the time between collisions; the local equilibrium value $\mathbf{M}^{\mathrm{eq}} = \mathbf{m}(x, t) \exp(-p^2/2)/\sqrt{2\pi}$. This is the equation that we now discuss.

For small times we can use a time expansion $\mathbf{M}(x, p, t) = \mathbf{M}^{(0)} + \mathbf{M}^{(1)} t + \mathbf{M}^{(2)} t^2/2 + \ldots$ and solve (11) to each time order. The spin distribution immediately after the $\pi/2$ pulse is unchanged, except that $\mathbf{M}^{(0)}(x, p)$ is perpendicular to $\mathbf{e}_{\parallel}$. The density profile $n(x)$ remains Gaussian, so that the Bohr frequency $\overline{\Omega}(x)$ does not vary in time. The effect of real collisions [right-hand side of (11)] is neglected since we are interested in small time behavior only. The result of this calculation is that $m_{\parallel}(x, t)$ starts as t^4 with $m_{\parallel}^{(4)}(x) = \epsilon g_{12}^{\epsilon} n(x) [\overline{\Omega}''(x) n(x) + \overline{\Omega}'(x) \times \{n'(x) - x n(x)\}]/2\hbar$ in dimensionless form. Using the fact that the density $n(x)$ remains Gaussian and restoring the units, we get

$$\frac{m_{\parallel}(x, t)}{n(x)} = \frac{n_2 - n_1}{n} = \frac{\epsilon g_{12}^{\epsilon} n}{\hbar\omega} \frac{\overline{\Omega}'' x_T^2 - 2\overline{\Omega}' x}{\omega} \frac{(\omega t)^4}{48}. \quad (12)$$

The first factor on the right-hand side is of the order of the dimensionless ISRE constant $g_{12} n(0)/\hbar\omega$. Since its value in the experiment of Ref. [1] is ~ 20, it is not surprising that species separation could be observed in a time smaller than the trap period. The second factor involves the spatial variations of $\overline{\Omega}(x)$; near the center of the trap, a positive curvature implies a positive $m_{\parallel}$ ($n_2 \geq n_1$), in accordance with the results of [1] ($\tau_{\mathrm{ex}}^{\mathrm{fwd}} < 0$). Inserting the values of the parameters of the experiment of [1] into (12) leads to significant species separation ($m_{\parallel} \sim n$) for ~ 25 ms, to be compared with the observed 30–50 ms.

The maximum of the phenomenon can also readily be understood. For short times, we have seen that positive velocities along x correspond to one sign for the transverse orientation, and conversely. For times greater than $2\pi/\sqrt{\omega\,\delta\Omega}$ [$\delta\Omega$ is the variation of $\overline{\Omega}(x)$ between the center and the edge of the cloud], both velocity signs become correlated to all spin directions in the transverse plane, so that the apparent segregation effect averages out to zero. Typical values taken from the experiment of [1] give ~ 100 ms for the maximum of the phenomenon.

When, eventually, two separated species recombine under the effect of the restoring force of the trap, the ISRE plays no role anymore. The reason is merely that the operator associated with transverse spin is diagonal in the position representation (but not in the spin space), so that it can have nonzero value only if the wave packets associated with each internal state overlap. In the absence of transverse polarization, the system is equivalent to a classical mixture of two gases.

Numerically, Eq. (11) can be solved by propagating the initial distribution in time with the Lax-Wendroff method (see, e.g., [14]), with parameters taken from Ref. [1]. The Bohr frequency $\overline{\Omega}(x)$ is taken to be an inverted Gaussian of depth $\delta\Omega$ and half width x_T. The dimensionless ISRE constant is $g_{12} n(0)/\hbar\omega = 20$. The relaxation time is $\tau_M \sim 10$ ms [1], so that $\omega\tau_M \simeq 0.3$. The time evolution of the spin polarization at the center of the trap $\mathbf{m}(0, t)$ is shown in Fig. 1, with no adjustable parameter. The longitudinal spin polarization rises as predicted by (12), reaches

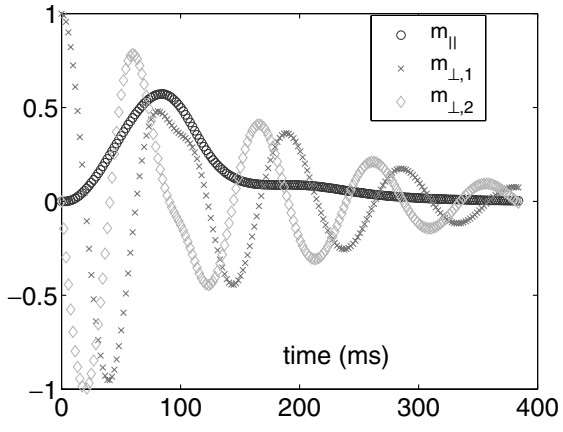

FIG. 1. Time evolution of the spin polarization $\mathbf{m}$ at the center of the trap; $m_{\parallel}$ corresponds to the population difference between the two states; $m_{\perp,1}$ and $m_{\perp,2}$ are the two components of the transverse spin polarization. The center-to-edge difference in Bohr frequency $\delta\Omega/2\pi$ is 12 Hz.

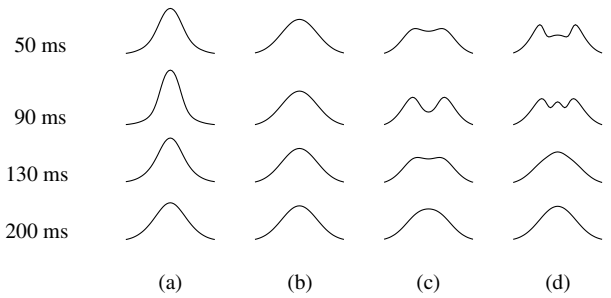

FIG. 2. Evolution of the particle density in state 1; $\delta\Omega/2\pi$ and $g_{12}n(0)/\hbar\omega$ are (a) -12 Hz, 20 (b) 0 Hz, 20 (c) 12 Hz, 20 (d) 30 Hz, 30. Note the good agreement with Fig. 3 of [1], including the sign of the effect and higher order effects.

a maximum around 90 ms, and then oscillates and decays to almost zero after 300 ms. Even in the pure Knudsen regime ($\tau_M = \infty$), a strong maximum of $m_\parallel$ is reached around 100 ms. Figure 1 also shows how the other components of the polarization oscillate and decay. An interesting feature of the experiment of Ref. [1] is that neither the hydrodynamic nor the collisionless regime is valid along the axis as $\omega\tau_M \sim 1$, so that a study of the full phase-space dynamics is necessary.

Figure 2 shows the time evolution of n_1 as a function of $\delta\Omega$, the variation of $\overline{\Omega}(x)$ between the center and the edge of the atomic cloud, and of $g_{12}n(0)/\hbar\omega$. When the curvature is zero [column (b)], no state separation occurs. Columns (a) and (c) show the effect of spin conversion for negative and positive curvature $\delta\Omega$ (at the center). For negative curvature, the atoms in state 1 are pulled towards the center of the trap, whereas for positive curvature they are expelled from it. Column (d) exhibits what authors of Ref. [1] call "higher order effects," for sufficiently large values of $\delta\Omega$ and $g_{12}n(0)/\hbar\omega$. These figures are in good qualitative agreement with Fig. 3 in Ref. [1].

In conclusion, the ISRE plays an important role in the dynamics of cold gases with internal states. In the experiment of Ref. [1], this effect creates large longitudinal spin oscillations in a nonhydrodynamic regime. Our calculations are also valid for fermions [15], where similar effects could be observed, in a case where $g_{11}^{\epsilon} = g_{22}^{\epsilon} = 0$ and the ISRE changes sign. Another interesting possibility is tuning the effect by changing g_{12}^{ϵ} at a Feshbach resonance [16]. Finally we note that, strictly speaking, our study is limited to nondegenerate gases; nevertheless, for noncondensed systems, most of the effect of degeneracy can be included by simply replacing the Maxwell-Boltzmann distribution by the appropriate quantum distribution [17], so that no dramatic change is expected.

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Note added.—While this Letter was being written, we became aware of the work of Oktel and Levitov [18], who reach conclusions similar to ours. Nevertheless, they use a hydrodynamic expression for the evolution of the spin current, while here we put more emphasis on the intermediate and Knudsen regimes.

*Email address: fuchs@lkb.ens.fr
†Email address: gangardt@lkb.ens.fr
‡Also at Department of Physics, Technion, 32000 Haifa, Israel.
§Email address: laloe@lkb.ens.fr

[1] H. J. Lewandowski, D. M. Harber, D. L. Whitaker, and E. A. Cornell, cond-mat/0109476.
[2] C. Lhuillier and F. Laloë, J. Phys. (Paris) **43**, 197 (1982).
[3] C. Lhuillier and F. Laloë, J. Phys. (Paris) **43**, 225 (1982); Phys. Rev. Lett. **54**, 1207 (1985).
[4] A. J. Leggett, J. Phys. C **3**, 448 (1970).
[5] E. P. Bashkin, JETP Lett. **33**, 8 (1981); JETP **60**, 1122 (1984); Sov. Phys. Usp. **29**, 238 (1986).
[6] L. Lévy and A. Ruckenstein, Phys. Rev. Lett. **52**, 1512 (1984).
[7] B. R. Johnson, J. S. Denker, N. Bigelow, L. P. Lévy, J. H. Freed, and D. M. Lee, Phys. Rev. Lett. **52**, 1508 (1984).
[8] G. Tastevin, P. J. Nacher, M. Leduc, and F. Laloë, J. Phys. Lett. **46**, 249 (1985).
[9] W. J. Gully and W. J. Mullin, Phys. Rev. Lett. **52**, 1810 (1984).
[10] F. Laloë and W. J. Mullin, J. Stat. Phys. **59**, 725 (1990).
[11] A. E. Meyerovich, Phys. Rev. B **39**, 9318 (1989).
[12] All the microscopic processes are purely elastic.
[13] L. S. Levitov (private communication); see also [18].
[14] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1986), Chap. 17.
[15] B. DeMarco and D. S. Jin, cond-mat/0109098.
[16] E. G. M. van Kempen, S. J. J. M. F. Kokkelmans, D. J. Heinzen, and B. J. Verhaar, cond-mat/0110610; T. Loftus, C. A. Regal, C. Ticknor, J. L. Bohn, and D. S. Jin, cond-mat/0111571.
[17] W. J. Mullin and J. W. Jeon, J. Low Temp. Phys. **88**, 433 (1992); K. Miyake, W. J. Mullin, and P. C. Stamp, J. Phys. (Paris) **46**, 663 (1985).
[18] M. Ö. Oktel and L. S. Levitov, preceding Letter, Phys. Rev. Lett. **88**, 230403 (2002).