Nonadiabatic dynamics of atoms in nonuniform magnetic fields

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Dynamics of neutral atoms in nonuniform magnetic fields, typical of quadrupole magnetic traps, is considered by applying an accurate method for solving nonlinear systems of differential equations. This method is more general than the adiabatic approximation and, thus, permits one to check the limits of the latter and also to analyze nonadiabatic regimes of motion. An unusual nonadiabatic regime is found when atoms are confined from one side of the z axis but are not confined from another side. The lifetime of atoms in a trap in this semiconfining regime can be sufficiently long for accomplishing experiments with a cloud of such atoms. At low temperature, the cloud is ellipsoidal, being stretched in the axial direction and moving along the z axis. The possibility of employing the semiconfining regime for studying the relative motion of one component through another in a binary mixture of gases is discussed. [S1050-2947(97)06412-3]

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I. INTRODUCTION

The motion of neutral atoms in nonuniform magnetic fields is important to study for several applications, in particular, for better understanding the mechanics of confinement in quadrupole magnetic traps, such as the Ioffe-Pritchard traps with a static bottle field [1-3] or dynamic traps with a rotating bias field [4,5]. This has become especially interesting after the experimental observation of Bose condensation in very cold gases of rubidium [6,7], lithium [8], and sodium [9-11]. There exists extensive literature considering statistical properties of confined Bose systems, using various approaches, e.g., the quasiclassical density-ofstate approximation [12,13], the Gross-Pitaevskii equation [14–16], the Monte Carlo density-matrix calculations [17], the Thomas-Fermi approximation [18,19], the Bogoliubov approximation [20], and the gas approximation in the framework of the Gibbs ensembles [21,22]. Statistical properties of the weakly interacting Fermi gas confined in a potential well have also been studied in the Thomas-Fermi approximation [23,24].

The aim of this paper is to consider not statistics but dynamics of atoms in nonuniform magnetic fields. When one is interested in the behavior of confined atoms, one deals with their stationary motion. Stationary regimes can be described by the adiabatic approximation. When the confining potential is harmonic, then the dynamics of atoms is given by simple harmonic oscillations. In general, the confining potential is not necessarily harmonic. For instance, the first demonstrated magnetic trap [25] used a quadrupole field (with zero magnetic field at the center) which gave rise to a linear potential. In any case, atomic motion in a strictly confining potential can be described by the adiabatic approximation. Such adiabatic motion in various magnetic traps has been analyzed in Refs. [26–29].

A more general consideration of atomic motion, without using the adiabatic approximation, is meaningful for several reasons: First of all, a more general approach makes it possible to understand the limits of the adiabatic approximation. Second, studying other, nonadiabatic, regimes of motion permits one to explain more profoundly the physics of atoms inside magnetic traps, as far as in these not all atoms are confined. Knowing better different, including nonadiabatic, regimes of atomic motion may, possibly, give a hint on how to improve confining characteristics of magnetic traps.

One more reason is related to the recently reported experiments on the simultaneous trapping of two different atomic species, two isotopes of rubidium [30] and sodium and potassium [31]. These experiments are a starting point for a new series of studies of ultracold matter. The variety of effects that can be observed in mixtures are incomparably richer than in one-component gases. This concerns even equilibrium mixtures [32]. Much more interesting features appear when one of the components can move through another. For instance, in a binary mixture with such a relative motion the effect of conical stratification [33] can occur. This effect happens when one of the components moves in one direction through another component. Then the instability can develop inside a cone with the axis along the relative velocity; as a result of this instability, the components stratify in space. Note that for this effect the one-directional relative motion is necessary, but not relative oscillations or collisions of sloshing clouds. In the presence of a relative macroscopic motion some unusual manifestations of the Doppler effect [34] may also arise. But can such a strange regime exist when the atoms of one kind move in one direction being confined from another? In addition, it is desirable that this one-directional escape from a trap would not be too fast in order to be able to accomplish measurements. These requirements look too severe to allow the existence of such a semiconfining regime. However, in what follows it will be shown that this semiconfining regime does exist. Certainly, it is nonadiabatic and, even more, nonpotential, thus cannot be described in the framework of the adiabatic approximation.

II. EVOLUTION EQUATIONS

Since the aim of this paper is to present an accurate solution of evolution equations for atoms in nonuniform mag-

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netic fields, it is reasonable, first of all, to pay attention to the accurate formulation of the equations themselves.

The quantum Hamiltonian of a system of N neutral atoms, each with a mass m and magnetic moment μ , is

$$H = \sum_{i=1}^{N} \left(\frac{\vec{p}_{i}^{2}}{2m} - \mu \vec{S}_{i} \vec{B}_{i} \right) + \frac{1}{2} \sum_{i \neq j}^{N} \Phi_{ij}, \qquad (1)$$

where \vec{p}_i is a momentum operator; \vec{S}_i , a spin operator; $\vec{B}_i = \vec{B}(\vec{r}_i, t)$ is the total magnetic field acting on an *i* atom; and $\Phi_{ij} = \Phi(|\vec{r}_i - \vec{r}_j|)$ is an interaction potential. The magnetic moment μ is the product of the Bohr magneton and the hyperfine *g* factor [35]. The wave function of the system, $\Psi = [\Psi_s(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)]$, is a column in spin space. The quantum-mechanical average of an operator from the algebra of observables, \mathcal{A} , is the scalar product

$$\langle \mathcal{A} \rangle = (\Psi, \mathcal{A}\Psi).$$
 (2)

Using the Schrödinger equation $i\hbar \partial \Psi / \partial t = H\Psi$, with the Hamiltonian (1), it is straightforward to get the evolution equations for the average position of an atom,

$$\frac{d}{dt}\langle \vec{r_i} \rangle = \frac{1}{m} \langle \vec{p_i} \rangle, \qquad (3)$$

its average momentum

$$\frac{d}{dt}\langle \vec{p}_i \rangle = \mu \langle \vec{\nabla}_i (\vec{S}_i \cdot \vec{B}_i) \rangle - \sum_{j(\neq i)}^N \langle \vec{\nabla}_i \Phi_{ij} \rangle, \qquad (4)$$

and the average spin

$$\frac{d}{dt}\langle \vec{S}_i \rangle = \frac{\mu}{\hbar} \langle \vec{S}_i \times \vec{B}_i \rangle.$$
(5)

These equations may be simplified with a mean-field approximation

$$\langle S_i^{\alpha} B_i^{\beta} \rangle = \langle S_i^{\alpha} \rangle \langle B_i^{\beta} \rangle, \tag{6}$$

where $\alpha, \beta = x, y, z$, valid for fields slowly varying in space [35]. Condition (6) is also called the semiclassical approximation and is usually supplemented by another approximate equation

$$\langle \vec{B}(\vec{r}_i,t) \rangle = \vec{B}(\langle \vec{r}_i \rangle,t), \tag{7}$$

which again assumes a slow variance of magnetic field in space. When the magnetic field is a linear function of real-space coordinates, then Eq. (7) is not an approximation but an exact relation. This concerns quadrupole magnetic fields which in what follows we shall deal with. Hence the sole approximation we need is the mean-field one, Eq. (6).

Under conditions (6) and (7), Eqs. (3)–(5) acquire the same form for all indices i, which permits us to simplify the notation by introducing

$$\vec{r} \equiv \langle \vec{r}_i \rangle = \{x, y, z\},\$$

$$\vec{v} \equiv \frac{1}{m} \langle \vec{p}_i \rangle = \{ v_x, v_y, v_z \}, \qquad (8)$$
$$\vec{S} \equiv \langle \vec{S}_i \rangle = \{ S_x, S_y, S_z \},$$

and the average interatomic force

$$\vec{f} \equiv -\sum_{j(\neq i)}^{N} \langle \vec{\nabla} \Phi_{ij} \rangle. \tag{9}$$

Then Eqs. (3)–(5) can be reduced to the system of equations

$$\frac{dr}{dt} = \vec{v},$$

$$\frac{d\vec{v}}{dt} = \frac{\mu}{m} \vec{\nabla} (\vec{S} \cdot \vec{B}) + \frac{\vec{f}}{m},$$
(10)
$$\frac{d\vec{S}}{dt} = \frac{\mu}{\hbar} \vec{S} \times \vec{B},$$

which will be the main object of our consideration.

The derivation of Eq. (10), though simple enough, contains an important point which is worth emphasizing. The basic approximation (6) supposes that the system fields slowly vary in real space, so that the spin and real-space degrees of freedom can be separated, which in the quantummechanical language means that the wave function can be factorized into a product of spin and real-space wave functions [35]. This quantum-mechanical separation of variables, as will be shown in what follows, is closely related to their dynamical separation.

The evolution equations (10) are to be supplemented by the initial conditions

$$\vec{r}(0) = \vec{r}_0 = \{x_0, y_0, z_0\},\$$

$$\vec{v}(0) = \vec{v}_0 = \{v_0^x, v_0^y, v_0^z\},\qquad(11)$$

$$\vec{S}(0) = \vec{S}_0 = \{S_0^x, S_0^y, S_0^z\}.$$

In specifying the form of the magnetic field, let us take it as in the experiments [5-7] with dynamical quadrupole traps. Then the total magnetic field

$$\vec{B} = \vec{B}_1(\vec{r}) + \vec{B}_2(t) \tag{12}$$

is the sum of the quadrupole field

$$\vec{B}_{1}(\vec{r}) = B_{1}'(\vec{r} - 3z\vec{e}_{z})$$
(13)

and the rotating bias field

$$\vec{B}_2(t) = B_2(\vec{e}_x \cos\omega t + \vec{e}_y \sin\omega t), \qquad (14)$$

where e_{α} is a unit vector for $\alpha = x, y, z$.

The characteristic length

$$L \equiv \frac{B_2}{B_1'} \tag{15}$$

of the quadrupole-field nonuniformity corresponds to the radius of the field zero in the radial direction. This length defines approximately the upper limit for the radius of a trapped atomic cloud. Keeping this in mind, it is convenient to pass to dimensionless space variables measuring the components of the Cartesian vector $\vec{r} = \{x, y, z\}$ in units of *L*. Then we can profit from the inequality

$$|\vec{r}| < 1. \tag{16}$$

To return to dimensional space variables, we have to set $\vec{r} \rightarrow \vec{r}/L$.

We introduce the characteristic frequencies

$$\omega_1 \equiv \left(\frac{\mu B_1'}{mL}\right)^{1/2}, \quad \omega_2 \equiv \frac{\mu B_2}{\hbar} \tag{17}$$

of atomic and spin motions, respectively, and the collision rate γ defined by the ratio

$$\gamma \vec{\xi} = \frac{\vec{f}}{mL},\tag{18}$$

in which ξ is treated as a stochastic variable representing the interactions of atoms through their random collisions. A detailed definition of the variable ξ will be given in Sec. V and in the Appendix. Then from Eq. (10) we obtain the evolution equations for the space variable

$$\frac{d^2 \vec{r}}{dt^2} = \omega_1^2 (S_x \vec{e}_x + S_y \vec{e}_y - 2S_z \vec{e}_z) + \gamma \vec{\xi}$$
(19)

and for the spin variable

$$\frac{d\tilde{S}}{dt} = \omega_2 \hat{A}\vec{S},\tag{20}$$

where the matrix $\hat{A} = [A_{\alpha\beta}]$, with $\alpha, \beta = 1, 2, 3$, consists of the elements

$$A_{11} = A_{22} = A_{33} = 0,$$

$$A_{12} = -A_{21} = -2z,$$

$$A_{13} = -A_{31} = -y - \sin\omega t,$$

$$A_{23} = -A_{32} = x + \cos\omega t.$$

We are concerned about an accurate solution of the system (19) and (20) of nonlinear differential equations, without using the adiabatic approximation. At this point, to distinguish what is what, it is useful to say several words about the adiabatic approximation. Fortunately, this will not take too much space, since the latter approximation is rather trivial. First, one assumes that the dynamical process is close to its stationary state, so that it is admissible to set $d\vec{S}/dt=\vec{0}$. Then, from the third equation in Eq. (10) it follows that $\vec{S} \times \vec{B} = \vec{0}$. This means that the spin is aligned along \vec{B} , which can be written as $\vec{S} \cdot \vec{B} = S |\vec{B}|$. Thus one excludes the spin motion saying that spin adiabatically follows the magnetic

field. Using this, for the atomic space variable \vec{r} one gets the Newton equation with the adiabatic force

$$\vec{F}_a = S \mu \vec{\nabla} |\vec{B}|.$$

Assume that the field rotates much faster than the mechanical oscillations of atoms, but not so fast as to induce transitions in the Zeeman substructure. This means that $\omega_1 \ll \omega \ll \omega_2$. Then the adiabatic force can be averaged over the period $2\pi/\omega$ of the rotating bias field. Averaging this force and using Eq. (16), one gets

$$\langle \vec{F}_a \rangle_t \simeq \frac{m}{2} S \omega_1^2 (x \vec{e}_x + y \vec{e}_y + 8z \vec{e}_z),$$

which immediately yields the adiabatic potential

$$U_a \simeq -\frac{m}{4} S \omega_1^2 (x^2 + y^2 + 8z^2) + \text{const.}$$

This is a harmonic, although anisotropic, potential. The motion of atoms in such a potential is given by simple harmonic oscillations, if S < 0. When S = 0, atoms fly away ballistically and if S > 0, they escape by the exponential law. In both latter cases atoms escape from the trap in all directions. The ballistic flying away is isotropic. The exponential escape, because of the anisotropy of the adiabatic potential, is anisotropic: atoms escape faster along the axial direction than in the radial one; but anyway the symmetry with respect to the inversion $\vec{r} \rightarrow -\vec{r}$ is preserved.

III. SCALE SEPARATION

Return to the general equations (19) and (20). Written in the standard form, they compose a nonlinear dynamical system of the ninth order, that is, a system of nine nonlinear differential equations. It seems that it is impossible to solve this complicated system of equations without invoking a rough approximation like the adiabatic one. Nevertheless, these equations can be solved using the method of scale separation [36,37]. The mathematical foundation of this approach is based on the Krylov-Bogoliubov averaging method [38] and the Poincaré theory of generalized asymptotic expansions [39]. The method of scale separation was successfully applied to several intricate problems, such as the origin of self-organized spin superradiance in nuclear magnets [36], coherent radiation regimes of spin masers [40,41], and fast polarization reversal in proton targets used for studying beam scattering [42]. The accuracy of this approach has been confirmed by good agreement of its solutions with experimental data [43,44] and with computer simulations [45,46].

The first step of the method of scale separation [36,37] is to classify the functional variables of the problem, separating time scales. Fortunately, in the majority of interesting physical problems it is possible to separate relatively slow from relatively fast variables. In our case, such a separation is naturally related to the mean-field condition (6) used for deriving the evolution equations (19) and (20). As has been already discussed above, condition (6) assumes that the realspace nonuniformity in the system is, in some sense, small. Now we ascribe an exact meaning to this phrase concretizing in what sense the nonuniformity is small. The nonuniformity in the system is connected with the quadrupole field (13) and pair interactions in Eq. (9), while the rotating bias field (14) is spatially uniform. Therefore what we need is to compare the characteristic parameters related to the corresponding fields. Among these characteristic parameters we have ω_1 and ω_2 in Eq. (17), and γ in Eq. (18). The nonuniformity is weak if the characteristic parameters corresponding to nonuniform fields are small as compared to that of a uniform field. The latter means nothing but the validity of the inequalities

$$\omega_1 \ll \omega_2, \quad \gamma \ll \omega_2.$$
 (21)

The meaning of the first inequality in Eq. (21) is quite evident, indicating that the frequency of mechanical oscillations of atoms is much smaller than that of spin fluctuations. The second inequality is also very natural, as long as the collision rate is usually much smaller than ω_2 . If γ were comparable with ω_2 this would imply atomic collisions are causing radio-frequency transitions between magnetic sublevels. With Eq. (21) in mind, looking at the evolution equations (19) and (20), we notice at once that the variable \vec{S} .

At this point, it is worth emphasizing how naturally the separation of functional variables into slow and fast, with respect to time, is connected with the character of nonuniformity in real space. This is why spending some time for remembering the derivation of Eqs. (10) was not in vain, but, on the contrary, is important for stressing the self-consistency of the approximations used.

Following further the method of scale separation [36,37], we need to solve the equations for fast variables, with slow variables being kept as quasi-integrals of motion. The evolution equation for fast variables is Eq. (20) for spin. This equation for an arbitrary given antisymmetric matrix \hat{A} , with elements $A_{ij} = -A_{ji}$, can be solved exactly. This means that we are able to present an exact solution for \vec{S} for any given external fields. Because of the significance of such a solution, we write it down explicitly.

First, we solve the eigenproblem

$$\hat{A}\vec{b}_{i} = \alpha_{i}\vec{b}_{i}, \quad |\vec{b}_{i}|^{2} = 1,$$
 (22)

in which \hat{A} is an antisymmetric matrix and i=1,2,3. The solution is straightforward, giving the eigenvalues

$$\alpha_1 = i\alpha, \quad \alpha_2 = -i\alpha, \quad \alpha_3 = 0, \tag{23}$$

with

$$\alpha \equiv \sqrt{A_{12}^2 + A_{13}^2 + A_{23}^2}.$$

The eigenvectors are

$$\vec{b}_{i} = \frac{1}{\sqrt{C_{i}}} [(\alpha_{i}A_{13} + A_{12}A_{23})\vec{e}_{x} + (\alpha_{i}A_{23} - A_{12}A_{13})\vec{e}_{y} + (\alpha_{i}^{2} + A_{12}^{2})\vec{e}_{z}], \qquad (24)$$

with the normalization constant

$$C_i = (|\alpha_i|^2 - A_{12}^2)^2 + (|\alpha_i|^2 + A_{12}^2)(A_{13}^2 + A_{23}^2).$$

It can be checked straightaway that the vectors from Eq. (24) form an orthonormal basis and satisfy the properties

$$\vec{b}_i^* \cdot \vec{b}_j = \delta_{ij}, \quad \vec{b}_1^* = \vec{b}_2, \quad \vec{b}_3^* = \vec{b}_3.$$
 (25)

Therefore the general solution of Eq. (20) can be written as a linear combination

$$\vec{S}(t) = \sum_{i=1}^{3} a_i \vec{S}_i(t)$$
(26)

of particular solutions

$$\vec{S}_i(t) = \vec{b}_i(t) \exp\{\varphi_i(t)\},\tag{27}$$

in which \vec{b}_i are given by Eq. (24). The coefficients in Eq. (26) are defined by the initial condition for spin from Eq. (11), which yields

$$a_i = \tilde{S}_0 \cdot \tilde{b}_i^*(0).$$
 (28)

Substituting Eq. (27) into Eq. (20), we obtain the phase

$$\varphi_i(t) = \int_0^t \left[\omega_2 \alpha_i(t) - \vec{b}_i^*(t) \frac{d}{dt} \vec{b}_i(t) \right] dt.$$
 (29)

From Eq. (29), invoking Eq. (25), we find that

$$\varphi_1^* = -\varphi_1, \quad \varphi_2^* = -\varphi_2, \quad \varphi_3 = 0.$$
 (30)

Let us accent that, of course, not each system of equations like Eq. (20) can be solved exactly. The possibility of obtaining here the exact solution, Eq. (26), is due to the antisymmetry of the matrix \hat{A} .

IV. ATOMIC VARIABLES

At the next step of the method of scale separation [36,37] the solution for fast variables is to be substituted into the equations for slow variables with time averaging the right-hand side of the latter equations. As follows from Eqs. (27) and (29), the fast spin fluctuations are described by the effective time-dependent frequencies $\varphi_i(t)/t$. Hence the solution (26) does not have a definite period. Consequently, the time averaging is given by the rule

$$\langle F \rangle_t \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau F(t) dt.$$
 (31)

Averaging Eq. (26) according to the rule (31) and using Eq. (16), we find

$$\langle \vec{S} \rangle_t = \frac{1}{2} [(1+x)S_0^x + yS_0^y - 2zS_0^z] (x\vec{e}_x + y\vec{e}_y - 4z\vec{e}_z).$$
(32)

The equation for the guiding centers of atomic variables is obtained by time averaging the right-hand side of Eq. (19) with $\vec{\xi}$ treated as a slow variable. Employing Eq. (32), we have

$$\frac{d^2r}{dt^2} = \vec{F} + \gamma \vec{\xi},\tag{33}$$

with the force

$$\vec{F} = \frac{\omega_1^2}{2} [(1+x)S_0^x + yS_0^y - 2zS_0^z](x\vec{e}_x + y\vec{e}_y + 8z\vec{e}_z).$$
(34)

This force essentially depends on the initial polarization of spins, as it should be in the general case and in contrast to the adiabatic force mentioned at the end of Sec. II. Only for one type of initial polarization, when $S_0^x = S$ and $S_0^y = S_0^z = 0$, does the force (34) reduce to the adiabatic one. This type of spin polarization leads to the stationary confined motion for which the adiabatic approximation is admissible.

Let us analyze another situation when spins are initially polarized along the z axis, so that

$$S_0^x = 0, \quad S_0^y = 0, \quad S_0^z = S.$$
 (35)

Then the force (34) becomes

$$\vec{F} = -S\omega_1^2 z(\vec{r} + 7z\vec{e}_z).$$
(36)

As is evident, the force (36) is nonadiabatic and, even more, it is nonpotential since there exists no potential U such that \vec{F} would be equal to $-\vec{\nabla}U$.

With the force (36), Eq. (33) becomes

$$\frac{d^2 \vec{r}}{dt^2} + S \omega_1^2 z (\vec{r} + 7 z \vec{e}_z) = \gamma \vec{\xi}.$$
(37)

The force $\gamma \bar{\xi}$, according to Eq. (18), originates from interatomic interactions in Eq. (9). Because of the isotropy of the interaction potential $\Phi(|\vec{r_i} - \vec{r_j}|)$, the force corresponding to these interactions may be presented as an isotropic vector, that is, we may write

$$\vec{\xi} = \xi(\vec{e}_x + \vec{e}_y + \vec{e}_z).$$
 (38)

Expanding Eq. (37) into components, we get for the *x* component

$$\frac{d^2x}{dt^2} + S\omega_1^2 z x = \gamma \xi. \tag{39}$$

The equation for the y component is the same as Eq. (39) with the replacement $x \rightarrow y$. Therefore we shall consider in what follows only one of the radial components. For the axial variable, Eq. (37) gives

$$\frac{d^2z}{dt^2} + 8S\omega_1^2 z^2 = \gamma \xi. \tag{40}$$

So, we have to solve the system of nonlinear equations (39) and (40).

The general solutions to Eqs. (39) and (40) can be written in the form

$$x = x_1 + x_2, \quad z = z_1 + z_2, \tag{41}$$

in which x_1 and z_1 are the solutions to the corresponding homogeneous equations while x_2 and z_2 are the solutions to the nonhomogeneous equations. The homogeneous equations are

$$\frac{d^2 x_1}{dt^2} + S\omega_1^2 z_1 x_1 = 0,$$

$$\frac{d^2 z_1}{dt^2} + 8S\omega_1^2 z_1^2 = 0,$$
(42)

with the initial conditions

$$x_{1}(0) = x_{0}, \quad \dot{x}_{1}(0) = v_{0}^{x},$$

$$z_{1}(0) = z_{0}, \quad \dot{z}_{1}(0) = v_{0}^{z}, \quad (43)$$

where the dot means the time derivative. Writing down the nonhomogeneous equations, simplifying them a little, taking into account that the collision rate is typically an order of magnitude smaller than ω_1 , yields

$$\frac{d^2 x_2}{dt^2} + S \omega_1^2 z_1 x_2 = \gamma \xi - S \omega_1^2 x_1 z_2,$$
$$\frac{d^2 z_2}{dt^2} + 16S \omega_1^2 z_1 z_2 = \gamma \xi,$$
(44)

the initial conditions for Eq. (44) being

$$x_2(0)=0, \ \dot{x}_2(0)=0,$$

 $z_2(0)=0, \ \dot{z}_2(0)=0.$ (45)

To solve the system of equations (42) and (44), we have, first, to solve the equation for z_1 , then to substitute z_1 into the equation for x_1 , and to use the found x_1 and z_1 in Eq. (44).

V. SEMICONFINED MOTION

The system of equations in Eq. (42) for x_1 and z_1 is a system of two nonlinear differential equations of second order. However, these equations can be solved exactly.

Integrating once the second equation in Eq. (42), we get

$$\left(\frac{dz_1}{dt}\right)^2 = \frac{16}{3}S\omega_1^2(z_m^3 - z_1^3),\tag{46}$$

where z_m is an integration constant which can be found from the initial conditions in Eq. (43) yielding

$$z_m^3 = z_0^3 + \frac{3(v_0^z)^2}{16S\omega_1^2}.$$
(47)

Since the left-hand side in Eq. (46) is nonnegative, this implies that $z_m^3 \ge z_1^3$ if S > 0, and $z_m^3 \le z_1^3$ if S < 0, that is, z_m is the maximal value of z_1 for S > 0 and z_m is the minimal value of z_1 for S < 0,

We introduce a function

$$\mathcal{P} = -\frac{4}{3}S\omega_1^2 z_1, \qquad (49)$$

for which Eq. (46) transforms to

$$\left(\frac{d\mathcal{P}}{dt}\right)^2 = 4\mathcal{P}^3 - g_2\mathcal{P} - g_3, \qquad (50)$$

where

$$g_2 = 0, \quad g_3 = -\frac{256}{27} z_m^3 S^3 \omega_1^6.$$
 (51)

Equation (50) is the Weierstrass equation with the Weierstrass invariants in Eq. (51) and with the discriminant

$$\Delta \equiv g_2^3 - 27g_3^2 = -27g_3^2.$$

The solution of the Weierstrass equation (50) is the Weierstrass function $\mathcal{P}(t-t_0)$, where t_0 is an integration constant. The Weierstrass function is an elliptic function, that is, a doubly periodic function which is analytic, except at poles, and which has no singularities other than poles in the finite part of the complex plane. All properties of the Weierstrass functions are perfectly described in Refs. [47,48].

In this way, the solution of Eq. (46), and therefore of Eq. (42), reads

$$z_1(t) = -\frac{3}{4S\omega_1^2} \mathcal{P}(t-t_0).$$
 (52)

The integration constant t_0 is to be found from the initial condition in Eq. (43), which gives

$$3\mathcal{P}(t_0) = -4z_0 S\omega_1^2, \tag{53}$$

where we took into account that the Weierstrass function is an even function. When t tends to t_0 , then

$$z_1(t) \simeq -\frac{3}{4S\omega_1^2} \left[\frac{1}{(t-t_0)^2} + \frac{g_3}{28}(t-t_0)^4 \right].$$
 (54)

The general behavior of $z_1(t)$ is as follows. If S > 0, then, starting from z_0 , the value of $z_1(t)$ increases to z_m from Eq. (47), after which it decreases, diverging to $-\infty$ as $t \rightarrow t_0$. If S < 0, then $z_1(t)$ decreases to its minimal value z_m , after which it turns to the positive direction, increasing to $+\infty$ as $t \rightarrow t_0$.

Substituting solution (52) into the first of Eqs. (42), we have the equation

$$\frac{d^2x_1}{dt^2} = \frac{3}{4}\mathcal{P}(t-t_0)x_1 \tag{55}$$

for the radial motion. This is a Lamé equation of degree n = 1/2, which is defined by the relation n(n+1) = 3/4. The solution to the Lamé equation is given by combinations of Lamé functions of different kinds [49]. In the present case, the solution to Eq. (55) is

$$x_1(t) = \left[c_1 \mathcal{P}\left(\frac{t-t_0}{2}\right) + c_2\right] E_3^{-1/2} \left(\frac{t-t_0}{2}\right).$$
(56)

Here

$$E_3(t) \equiv \frac{d}{dt} \mathcal{P}(t)$$

is a Lamé function of degree 3, of the first kind. The integration constants c_1 and c_2 are defined by the initial conditions in Eq. (43).

The solution (56) diverges together with Eq. (52), as $t \rightarrow t_0$, by the law

$$x_1(t) \simeq c_1 \left(\frac{t-t_0}{2}\right)^{-1/2} + c_2 \left(\frac{t-t_0}{2}\right)^{3/2}.$$
 (57)

Comparing Eqs. (57) and (54), we see that the divergence along the axial direction is faster than in the radial one, the aspect ratio being

$$\sqrt{\frac{x_1^2(t)}{z_1^2(t)}} \sim |t - t_0|^{3/2}.$$
(58)

This ratio tends to zero, as $t \rightarrow t_0$. Therefore a cloud of atoms acquires an ellipsoidal shape stretched in the axial direction.

The behavior of $x_1(t)$ and $z_1(t)$ shows that the atoms with an initial polarization S>0 are confined from the side z>0but are not confined from the side z<0. Vice versa, the atoms with an initial polarization S<0 are confined from the side z<0 but are not confined from that z>0. Thus an ensemble of atoms, with a given polarization, loaded into a trap would move predominantly in one direction either to z<0 or to z>0 depending on whether the initial polarization is S>0or S<0, respectively. Such a regime is exactly that semiconfining regime we have been looking for.

However, we need yet to find the solutions of nonhomogeneous equations in Eq. (44). To this end, we have to concretize the variable ξ originating from the averaged pair interactions. For a rarefied system these interactions can be treated as random pair collisions. The system is said to be rarefied if the average atomic density ρ and the scattering length *a* satisfy the inequality $\rho a^3 \ll 1$. This is just the case of experiments [5–11] with alkali-metal atoms. Therefore we can consider ξ as a random variable. More accurately, $\xi(t)$ can be modeled by a stochastic field. The latter may be specified as white Gaussian noise [50] with the stochastic averages

$$\langle\langle \xi(t) \rangle\rangle = 0, \quad \langle\langle \xi(t)\xi(t') \rangle\rangle = 2D\,\delta(t-t'),$$
 (59)

where *D* is a diffusion rate, and the meaning of double brackets is explained in the Appendix. Then the nonhomogeneous equations in Eq. (44) become stochastic differential equations. An explicit way of treating the random variable ξ is presented in the Appendix.

When solving the nonhomogeneous equations, it is useful to invoke again the idea of scale separation. The time variation of solutions to stochastic differential equations reflects the properties of the given stochastic fields. Since in our case the stochastic field $\xi(t)$ is modeled by white noise, which is characterized by sharp time jumps [50], then the related functional variables x_2 and z_2 can be treated as fast compared to x_1 and z_1 satisfying the equations not containing such random fields. Hence for the stochastic differential equations in Eq. (44), the slow variables x_1 and z_1 can be kept as quasi-integrals of motion [36,37]. Then using the method of Laplace transforms, we obtain

$$x_{2}(t) = \int_{0}^{t} G_{x}(t-\tau) [\gamma \xi(\tau) - S\omega_{1}^{2}x_{1}z_{2}(\tau)]d\tau \qquad (60)$$

and

$$z_2(t) = \int_0^t G_z(t-\tau) \gamma \xi(\tau) d\tau, \qquad (61)$$

where the initial conditions in Eq. (45) have been taken into account, and the transfer functions are

$$G_x(t) = \frac{\sin(\varepsilon t)}{\varepsilon}, \quad G_z(t) = \frac{\sin(4\varepsilon t)}{4\varepsilon},$$

with the effective frequency

$$\varepsilon \equiv \sqrt{Sz_1}\omega_1.$$

Employing condition (59), we may find the moments of solutions (60) and (61). For instance,

$$\langle \langle x_2(t) \rangle \rangle = 0, \ \langle \langle z_2(t) \rangle \rangle = 0.$$
 (62)

Calculating the second moments, we get the mean-square deviations for the radial random variable,

$$\langle \langle x_2^2(t) \rangle \rangle = \frac{\gamma^2 Dt}{\varepsilon^2} \bigg[1 - \frac{\sin(2\varepsilon t)}{2\varepsilon t} \bigg] + \frac{\gamma^2 Dt x_1^2}{3600\varepsilon^2 z_1^2} \\ \times \bigg\{ 1 - \cos(\varepsilon t) \cos(4\varepsilon t) + \frac{\sin(4\varepsilon t)}{4\varepsilon t} \\ \times [\cos(\varepsilon t) - \cos(4\varepsilon t) - 16\varepsilon t \sin(\varepsilon t)] \bigg\}, \quad (63)$$

and for the axial random variable,

$$\langle \langle z_2^2(t) \rangle \rangle = \frac{\gamma^2 D t}{16\varepsilon^2} \bigg[1 - \frac{\sin(8\varepsilon t)}{8\varepsilon t} \bigg].$$
 (64)

Note that the collision rate γ enters here as γ^2 , thence the behavior of the random variables (63) and (64) does not depend on whether the interatomic interactions are repulsive or attractive.

When the variables x_1 and z_1 diverge as in Eqs. (56) and (54), then for the random variables in Eqs. (63) and (64) we obtain

$$\langle \langle x_2^2(t) \rangle \rangle = \propto |t - t_0|^6 \exp\left(\frac{4\sqrt{3}t}{|t - t_0|}\right),$$
$$\langle \langle z_2^2(t) \rangle \rangle = \propto |t - t_0|^3 \exp\left(\frac{4\sqrt{3}t}{|t - t_0|}\right),$$
(65)

as $t \rightarrow t_0$. Since this expansion is governed by the same exponentials, it is practically isotropic, with only a slight anisotropy due to different preexponential factors.

Remember that the general solutions to Eqs. (39) and (40) have the form of the sums in Eq. (41) containing both the regular terms x_1 and z_1 and the random terms x_2 and z_2 . The relative contribution of these terms is regulated by the relation between the parameters γ , D, and ω_1 . If $\gamma^2 D \ll \omega_1^3$, then the influence of the random terms x_2 and z_2 is negligibly small, and the atomic motion is characterized by the regular terms x_1 and z_1 . In this case we have the semiconfining regime. An ensemble of atoms would form an ellipsoidal cloud moving in one of the directions along the z axis. If $\gamma^2 D \gg \omega_1^3$, then the motion of atoms is governed by the random terms x_2 and z_2 . In such a case, an ensemble of atoms would form an almost isotropic exponentially expanding cloud.

Assuming, as usual, that the diffusion rate D is proportional to temperature T, we come to the conclusion that the realization of either the regime of the fast exponential expansion or the regime of the slow semiconfined motion depends on temperature. At high temperatures the former regime will be realized while at low temperatures, the latter. A crossover temperature T_c related to the equality $\gamma^2 D = \omega_1^3$ would correspond to the effective boundary between these two regimes.

VI. NUMERICAL ESTIMATES

In order to impart to the whole consideration a completely realistic flavor and to show the reasonableness of all inequalities assumed for employing the method of scale separation, let us adduce numerical estimates basing on the characteristic quantities typical of the experiments [5–7] with ⁸⁷Rb in dynamical quadrupole traps.

The mass of a rubidium atom is $m = 1.45 \times 10^{-22}$ g and the magnetic moment is $\mu = 0.45 \times 10^{-20}$ erg/G. The gradient of the quadrupole field is $B'_1 = 120$ G/cm, and the amplitude of the rotating bias field is $B_2 = 10$ G, the rotation frequency of the latter being $\omega \approx 5 \times 10^4$ s⁻¹. The nonuniformity length (15) is $L \sim 0.1$ cm. The characteristic frequency of atomic motion and the Larmor frequency of spins from Eq. (17) are $\omega_1 \sim 10^2$ s⁻¹ and $\omega_2 \sim 5 \times 10^7$ s⁻¹, respectively. The collision rate in Eq. (18) can be estimated as $\gamma \sim \hbar \rho a/m$, which, with the average density $\rho \approx 3 \times 10^{12}$ cm⁻³ and the scattering length $a \sim 10^{-6}$ cm, gives $\gamma \sim 10$ s⁻¹. Thus the following inequalities hold true: Hence the classification of atomic variables as slow and of spin variables as fast, based on the inequalities in Eq. (21), is correct.

To estimate the lifetime t_0 of the semiconfined motion described in Sec. V, we have to return to Eq. (50). Integrating this over time between t=0 and some t, we have

$$\int_{\mathcal{P}(t_0)}^{\mathcal{P}(t-t_0)} \frac{d\mathcal{P}}{\sqrt{4\mathcal{P}^3 - g_2\mathcal{P} - g_3}} = t$$

From here, taking into account that $g_2=0$ and $\mathcal{P}(t-t_0) \rightarrow \infty$, as $t \rightarrow t_0$, we get

$$t_0 = \int_{\mathcal{P}(t_0)}^{\infty} \frac{d\mathcal{P}}{\sqrt{4\mathcal{P}^3 - g_3}}.$$
 (66)

Comparing Eqs. (51) and (53), we find for the Weierstrass invariant

$$g_3 = 4 \left(\frac{z_m}{z_0}\right)^3 \mathcal{P}^3(t_0).$$

Then Eq. (66) can be rewritten as

$$t_0 = \tau_0 \int_{-\infty}^{z_0} \frac{dz}{\sqrt{z_m^3 - z^3}},\tag{67}$$

where we assume that S > 0 and

$$\tau_0 \equiv \frac{1}{4\omega_1} \sqrt{\frac{3}{S}}.$$

The value of z_m is given by Eq. (47). The average kinetic energy $1/2m(v_0^z)^2L^2$ can be expressed through temperature as $1/2k_BT$. Therefore Eq. (47) acquires the form

$$z_m^3 = z_0^3 + \zeta, (68)$$

in which

$$\zeta = \frac{3T}{16T_0}, \ T_0 = \frac{mS\omega_1^2 L^2}{k_B}.$$

Finally, for the lifetime (67) we obtain

$$t_0 = \tau_0 \int_{-z_0}^{\infty} \frac{dz}{\sqrt{z^3 + z_0^3 + \zeta}}.$$
 (69)

For the quantities considered, we have $\tau_0 \approx 10^{-2}s$ and $T_0 \approx 10^{-4}$ K. The parameter ζ depends on temperature. In the interval of temperatures between 1 nK and 1 mK, it changes from 10^{-6} to 1. The quantity z_0 , according to Eq. (43), is the initial coordinate $z_1(0)$. It is clear that a cloud of trapped atoms should have a distribution of z_0 which depends on the temperature and shape of the confining potential. The average value of z_0 can be interpreted as the initial location of the center of an atomic cloud. This value can be different for different experiments. Keeping this in mind, we consider below several values of z_0 . The integral (69) was calculated numerically for different initial positions z_0 . The results are presented in Table I. As is seen, for the temperatures

TABLE I. The characteristic time t_0 , in seconds, for several parameters ζ and different initial conditions.

ζ	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1
ζ0							
-0.1	0.08	0.07	0.07	0.06	0.05	0.04	0.03
-0.01	0.20	0.16	0.12	0.09	0.06	0.04	0.03
-0.001	0.27	0.19	0.13	0.09	0.06	0.04	0.03
0	0.28	0.19	0.13	0.09	0.06	0.04	0.03
0.001	0.29	0.19	0.13	0.09	0.06	0.04	0.03
0.01	0.33	0.22	0.14	0.09	0.06	0.04	0.03
0.1	0.13	0.13	0.12	0.10	0.07	0.04	0.03

tures $T \approx 10^{-5}$ K the time t_0 becomes of order 0.1 s, and for $T \approx 1$ nK it reaches $t_0 \approx 0.3$ s. Moreover, making the temperature lower, it is possible to make t_0 arbitrarily large, since $t_0 \rightarrow \infty$ when $\zeta \rightarrow 0$. Notice that the lifetime t_0 does not change much when varying z_0 in the interval $-0.1 \le z_0 \le 0.1$.

It is possible to pose the question: how well does the lifetime t_0 characterize the real escape time of an atom from a trap? Looking at Eq. (54), we see that $z_1(t)$ diverges as $t \rightarrow t_0$, while, according to condition (16), the actual escape of an atom from a trap occurs at the time t_1 , when $z(t_1) \sim 1$. The relation between the times t_0 and t_1 , as follows from Eq. (54), is $t_1 - t_0 \sim \omega_1^{-1}$. This, with the given $\omega_1 \sim 10^2 \text{ s}^{-1}$, makes $t_1 - t_0 \sim 10^{-2} \text{ s}$. So, if $t_0 \ge 0.1 \text{ s}$, then $t_1 \sim t_0$. Therefore the time t_0 really plays the role of the average lifetime of atoms in a trap during the regime of semiconfined motion.

If we are not satisfied by the simple estimates for the characteristic time t_1 , we can calculate it *exactly* from the equation of motion. The procedure is the same as that for calculating t_0 . The results of this calculation confirm that t_1 is very close to the time t_0 , being smaller by about 0.02 s. Because of the mutual closeness of these times, we do not repeat for t_1 the whole table as for t_0 but, for cogency, we present in Table II the values of t_1 for the particles with the initial location at the center of the trap. These values are found from the formula

$$t_1 = \tau_0 \int_0^1 \frac{dz}{\sqrt{z^3 + \zeta}}.$$
 (70)

Similarly to t_0 , the time t_1 also becomes arbitrarily large, $t_1 \rightarrow \infty$, as $\zeta \rightarrow 0$, i.e., when temperature decreases.

Treating the interactions of atoms as random pair collisions is admissible if the atomic system is rarefied, so that $\rho a^3 \ll 1$. For the case considered, $\rho \sim 10^{12}$ cm⁻³ and $a \sim 10^{-6}$ cm, yielding $\rho a^3 \sim 10^{-6}$. Thus the assumed inequality is well satisfied.

As is argued at the end of Sec. V, at high temperatures there exists a regime of fast exponential expansion of an almost isotropic cloud. At low temperatures, the regime

TABLE II. The characteristic time t_1 , in seconds, for the atoms initially located at the center of the trap and for different parameters ζ .

ζ	10 ⁻⁶	10 ⁻⁵	10^{-4}	10 ⁻³	10^{-2}	10^{-1}	1
<i>t</i> ₁	0.26	0.17	0.11	0.07	0.04	0.02	0.01

changes to the semiconfined motion of a slowly moving ellipsoidal cloud. The crossover temperature T_c can be defined by the equality $\gamma^2 D = \omega_1^3$. The latter, with the diffusion rate $D \sim k_B T/\hbar$, gives

$$T_c \sim \frac{\hbar \omega_1^3}{k_B \gamma^2}.$$

Substituting here $\omega_1 \sim 10^2$ s⁻¹ and $\gamma \sim 10$ s⁻¹, we have $T_c \sim 10^{-7}$ K, which is close to the temperature of the Bose condensation observed in experiments [6,7]. Consequently, the semiconfined regime can also be realized under similar conditions.

Keeping in mind the future possibility of applying statistical methods to describe an ensemble of atoms in the semiconfining regime, we have to understand whether the local equilibrium can be established in this case. The time of local equilibrium is related to the collision rate as $\tau_{\rm loc} \sim \gamma^{-1}$. Hence for $\gamma \sim 10 \text{ s}^{-1}$, we have $\tau_{\text{loc}} \sim 0.1 \text{ s}$. The local equilibrium develops if the lifetime of the cloud, t_0 , is longer than the local-equilibrium time. If $t_0 \sim 0.3$ s, then the local equilibrium can be achieved. Of course, the global equilibrium for a semiconfined motion cannot exist. Recall that the corresponding force (36) is not confining for a semiaxis of z, and furthermore it is not potential. But the possibility of local equilibrium implies that a statistical description for such a regime can be done, e.g., with the help of hydrodynamic equations. If the local equilibrium is absent, one has to use kinetic equations.

VII. CONCLUSION

The method of scale separation is applied to the dynamics of neutral atoms in nonuniform magnetic fields typical of quadrupole magnetic traps. We concentrate our attention on the case of a dynamic quadrupole trap with a rotating bias field, as in experiments [5–7]. For the initial spin polarization $S_0^x < 0$, the motion of atoms is confined and well described by the adiabatic approximation.

For the atoms whose spins are initially polarized along the z axis a novel unusual regime appears where the motion is confined in a half space: when $S_0^z > 0$, the motion is confined from the side z>0, and if $S_0^z<0$, it is confined from the side z<0. This semiconfined motion is nonadiabatic and nonpotential. An ensemble of atoms in a semiconfining regime forms an ellipsoidal cloud stretched in the axial direction and slowly moving along the z axis to the nonconfining side.

The semiconfining regime can be used for studying mixtures with a relative motion of components. For example, one component can have initial spin polarization $S_0^x < 0$, thus, being confined, while another component, with initial spin polarization along the *z* axis, can be semiconfined, moving through the first. Or one can load into a trap two components both being polarized along the *z* axis, but one with $S_0^z > 0$ while another with $S_0^z < 0$. Then both such species will be in the semiconfining regime but moving in opposite directions, one to the negative *z* and another to positive *z* direction. The variant with three components, one of which is confined with the two others semiconfined moving in opposite directions, could also be realized. Mixtures with the relative motion of The semiconfining regime can also be employed for separating the species with different initial polarizations. For instance, if one loads into a trap a mixture of two components, one having the spin polarization up and another down, then the trap will act as a separator moving the first component down and the second one up, thus separating them.

One more application of the semiconfining regime could be for realizing atom lasers, for which a directed motion of atoms is necessary.

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APPENDIX: RANDOM VARIABLES

The variable $\xi(t)$ describing random pair collisions of atoms has been treated as a stochastic variable. Consequently, Eqs. (44) are stochastic differential equations. To find their solution, it was necessary to define the stochastic averages (59). The explicit definition of the random variable $\xi(t)$ and of the corresponding stochastic averages can be done in the following way.

Assume that there is a set $\{\varphi_n(t)\}$ of functions $\varphi_n(t)$ enumerated by a multi-index *n*. Let this set be complete and orthonormal,

$$\sum_{n} \varphi_{n}^{*}(t)\varphi_{n}(t') = \delta(t-t'), \quad \int \varphi_{m}^{*}(t)\varphi_{n}(t)dt = \delta_{mn}.$$

Then a function $\xi(t)$ can be represented as an expansion

$$\xi(t) = \sum_{n} \xi_{n} \varphi_{n}(t).$$

Each coefficient ξ_n is considered as a random variable with a probability distribution $p(\xi_n)$. For concreteness, we may think of $p_n(\xi_n)$ as a Gaussian distribution.

The stochastic averaging for a function $F(\xi(t))$ of the stochastic variable $\xi(t)$ is defined as the functional integral

$$\langle\langle F(\xi(t))\rangle\rangle = \int F(\xi(t))\prod_n p_n(\xi_n)d\xi_n$$

If the random coefficient ξ_n is complex, then $d\xi_n \equiv d(\operatorname{Re} \xi_n) d(\operatorname{Im} \xi_n)$. When ξ_n is centered at zero, then

$$\langle\langle \xi_n \rangle\rangle = \int \xi_n p_n(\xi_n) d\xi_n = 0.$$

The dispersion σ_n of a distribution $p_n(\xi_n)$ is given by the equation

$$\sigma_n^2 \equiv \langle \langle |\xi_n|^2 \rangle \rangle = \int |\xi_n|^2 p_n(\xi_n) d\xi_n$$

With these definitions, for the stochastic correlation function we have

$$\langle\langle \xi^*(t)\xi(t')\rangle\rangle = \sum_n \sigma_n^2 \varphi_n^*(t)\varphi_n(t')$$

In the case of white noise, all dispersions σ_n are equal to each other, so that we may write $\sigma_n^2 = 2D$. Thence the stochastic correlation function becomes

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$$\langle\langle \xi(t)\xi(t')\rangle\rangle = 2D\sum_{n} \varphi_{n}^{*}(t)\varphi_{n}(t'),$$

where it is taken into account that $\xi(t)$ is real. From here, because of the completeness of the basis $\{\varphi_n(t)\}$, we obtain Eq. (59) which was used in calculating expressions (62)–(65).

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