Nonadiabatic Regimes of Atomic Motion in Magnetic Traps

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The motion of neutral atoms in quadrupole magnetic traps is considered using an accurate method for solving nonlinear systems of differential equations. This approach, called the method of scale separation, does not involve the adiabatic approximation, thus, allows to analyze nonadiabatic regimes of motion. A new regime is found when atoms are confined from one side of a trap but are not confined from another side. Possible experimental applications of the semi-confining regime are discussed.

I. Introduction

The properties of neutral atoms in magnetic traps have recently attracted much attention in connection with the realization of the Bose condensation of alkali atoms (see review[1]). The motion of trapped atoms, as is generally believed, can be described in the adiabatic approximation. Although it has been argued that trapping can also occur in a nonadiabatic regime of resonant cooling[2]. What is certainly true is that in the more general picture, when atoms are permitted to escape from the trap, one has to give up the adiabatic approximation.

The aim of the present paper is to give an accurate solution to the equations of motion for neutral atoms in quadrupole magnetic traps, without using the adiabatic approximation. For this purpose, the *method of scale separation*[3−5] will be applied. The mathematical foundation of this approach is based on the Krylov–Bogolubov averaging method[6]. The method of scale separation has been successfully employed for describing dynamical processes in spin mazers[4,7,8], polarized targets[9], and nuclear magnets[5,10]. Its accuracy was confirmed by good agreement of found solutions with experimental data[11,12] and with computer simulations[13−15].

II. Basic Equations

The dynamics of neutral atoms in magnetic fields can be described in the semi–classical approximation which presupposes that the space variation of the magnetic fields is sufficiently slow, so that the spin and real–space degrees of freedom can be separated. In the quantum–mechanical language this means that the wave function can be factorized into a product of a spin and a real–space wave functions[16].

The equations of motion in the semi–classical approximation are

$$\frac{d^2\,\vec{r}}{dt^2} = \frac{\mu}{m}\,\vec{\nabla}\,(\vec{S}\vec{B}) + \frac{\vec{f}}{m} \tag{1}$$

for the real–space variable $\vec{r} = \{x, y, z\}$, and

$$\frac{d\,\vec{S}}{dt} = \frac{\mu}{\hbar}\,\vec{S}\times\vec{B} \tag{2}$$

for the spin variable $\vec{S} = \{S_x, S_y, S_z\}$. Here m is a mass of an atom and μ is the magnetic moment, that is, the product of the Bohr magneton and the hyperfine g –factor. The vector $\vec{f}$ in (1) represents the average force

$$\vec{f} = -\sum_{j(\neq i)}^{N}\langle\vec{\nabla}\,\Phi_{ij}\rangle, \tag{3}$$

with $\langle \ldots \rangle$ meaning the quantum–mechanical averaging, acting on an atom from other $N-1$ atoms interacting through the potential Φ_{ij} . The total magnetic field is $\vec{B}$. The evolution equations (1) and (2) are to be complimented by the initial conditions

$$\vec{r}\ (0) = \{x_0, y_0, z_0\},$$
$$\vec{v}\ (0) = \{v_0^x, v_0^y, v_0^z\}, \tag{4}$$
$$\vec{S}\ (0) = \{S_0^x, S_0^y, S_0^z\},$$

in which $\vec{v}\ (0) \equiv d\ \vec{r}\ /dt$ at $t = 0$.

The total magnetic field

$$\vec{B} = \vec{B}_1\ (\vec{r}) + \vec{B}_2\ (t) + \vec{B}_3\ (t) \tag{5}$$

consists of three parts: The first is the quadrupole field

$$\vec{B}_1\ (\vec{r}) = B_1'(\vec{r}\ - 3z\ \vec{e}_z) \tag{6}$$

typical of quadrupole magnetic traps, such as the Ioffe–Pritchard traps with a static bottle field[17−19] or dynamical traps with a rotating bias field[20,21]. The second term in (5) is the rotating bias field

$$\vec{B}_2\ (t) = B_2(\vec{e}_x\ \cos\omega t + \vec{e}_y\ \sin\omega t), \tag{7}$$

as in the dynamic trap[21]. Finally, the third term is a cooling radio–frequency field

$$\vec{B}_3\ (t) = B_3\ \vec{e}_z\ \cos\omega_r t \tag{8}$$

serving for removing fast particles from the trap.

For what follows, it is convenient to deal with the dimensionless space variable $\vec{r}$ measured in units of the characteristic length

$$L \equiv \frac{B_2}{B_1'}. \tag{9}$$

The latter roughly defines the linear size of the atomic cloud in a trap. Therefore, in dimensionless units we have

$$|\ \vec{r}\ | < 1. \tag{10}$$

To return to the dimensional space variable, we need to put $\vec{r} \rightarrow \vec{r}\ L$.

Define the characteristic frequencies

$$\omega_1 \equiv \sqrt{\frac{\mu B_1'}{mL}}, \qquad \omega_2 \equiv \frac{\mu B_2}{\hbar} \tag{11}$$

of atomic and spin motions, respectively, and use the notation

$$\zeta \equiv \frac{\omega_3}{\omega_2}, \qquad \omega_3 \equiv \frac{\mu B_3}{\hbar}. \tag{12}$$

Also, introduce the collision rate γ given by the relation

$$\gamma\ \vec{\xi} \equiv \frac{\vec{f}}{mL}. \tag{13}$$

In what follows we shall treat $\vec{\xi}$ as a random variable.

Then, Eq.(1) for the space variable takes the form

$$\frac{d^2\ \vec{r}}{dt^2} = \omega_1^2(S_x\ \vec{e}_x + S_y\ \vec{e}_y - 2S_z\ \vec{e}_z) + \gamma\ \vec{\xi}; \tag{14}$$

and Eq.(2) for the spin variable can be written as

$$\frac{d\ \vec{S}}{dt} = \omega_2 \hat{A}\ \vec{S}, \tag{15}$$

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

$$A_{11} = A_{22} = A_{33} = 0,$$
$$A_{12} = -A_{21} = -2z + \zeta\cos\omega_r t,$$
$$A_{13} = -A_{31} = -y - \sin\omega t,$$
$$A_{23} = -A_{32} = x + \cos\omega t.$$

Eqs.(14) and (15) are the basic evolution equations to be considered.

III. Scale Separation

To apply the method of scale separation[3−5] for solving the system of nonlinear equations (14) and (15), let us take the characteristic parameters as in experiments[21,22]. Then $\omega_1 \sim 10^2 s^{-1}$, $\omega_2 \sim 5 \times 10^7 s^{-1}$, the value of ω_3 may be somewhere in the interval between zero and $10^6 s^{-1}$, $\omega \sim 5 \times 10^4 s^{-1}$, ω_r is of the order of ω_2 and $\gamma \sim 1\ s^{-1} - 10\ s^{-1}$. Thus, the following sequence of inequalities holds:

$$\gamma \ll \omega_1 \ll \omega \ll \omega_2, \tag{16}$$

with $\omega_3 \ll \omega_2$ and $\omega_r \sim \omega_2$.

The inequalities in (16) show thath the space variables can be treated as slow while the spin variables as fast. Therefore, the former can be considered as the quasi–integrals of motion for the latter. Eq.(15), under fixed $\vec{r}$, can be solved exactly, and the solution writes

$$\vec{S}\ (t) = \sum_{i=1}^{3} a_i\ \vec{S}_i\ (t), \tag{17}$$

where

$$a_i = \vec{S}_0 \vec{b}_i^{\,*}(0), \qquad \vec{S}_0 \equiv \vec{S}(0),$$

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

$$\vec{b}_i(t) = \frac{1}{\sqrt{C_i}} \left[(\alpha_i A_{13} + A_{12}A_{23}) \vec{e}_x + (\alpha_i A_{23} - A_{12}A_{13}) \vec{e}_y + (\alpha_i^2 + A_{12}^2) \vec{e}_z \right],$$

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

$$\alpha_1 = i\alpha, \qquad \alpha_2 = -i\alpha, \qquad \alpha_3 = 0, \qquad \alpha \equiv \sqrt{A_{12}^2 + A_{13}^2 + A_{23}^2},$$

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

Substitute the solution (17) into Eq.(14) averaging the right–hand side of the latter according to the rule

$$\bar{F} \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau F(t) dt. \tag{18}$$

Take into account that $\omega_3 \ll \omega_2$, so $\zeta \ll 1$, and make use of the inequality (10). Then Eq.(14) reduces to

$$\frac{d^2 \vec{r}}{dt^2} = \vec{F} + \gamma \vec{\xi}, \tag{19}$$

with the force

$$\vec{F} = \frac{\omega_1^2}{2} [(1+x)S_0^x + yS_0^y + (\zeta - 2z)S_0^z] (x \vec{e}_x + y \vec{e}_y + 8z \vec{e}_z). \tag{20}$$

If initial conditions are such that $S_0^x = S$ and $S_0^y = S_0^z = 0$, then (20) trivializes to the adiabatic force

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

In the latter case, atoms are confined inside the trap for $S < 0$ and unconfined for $S > 0$ or $S = 0$.

IV. Nonadiabatic Motion

Consider nonadiabatic motion with the initial conditions for the spin variables in the form

$$S_0^x = 0, \qquad S_0^y = 0, \qquad S_0^z = S. \tag{21}$$

Because of the isotropy of the interaction potential, the force of interatomic interactions is to be an isotropic vector, so that for the corresponding random variable describing atomic collisions we may write

$$\vec{\xi} = \xi(\vec{e}_x + \vec{e}_y + \vec{e}_z). \tag{22}$$

Under these conditions, from Eq.(19) we have for the variable x the equation

$$\frac{d^2x}{dt^2} + S\omega_1^2 \left(z - \frac{\zeta}{2} \right) x = \gamma\xi. \tag{23}$$

The same equation, with the replacement of x by y , follows for the variable y . And for z we get

$$\frac{d^2z}{dt^2} + 8S\omega_1^2 \left(z - \frac{\zeta}{2} \right) z = \gamma\xi. \tag{24}$$

If ζ is not too small, there can appear oscillatory solutions when atoms oscillate about the point $\zeta/2$. This can be shown by putting

$$u = z - \frac{\zeta}{2}, \qquad |u| \ll 1,$$

and linearizing Eq.(24), which results in the equation

$$\frac{d^2u}{dt^2} + \omega_{eff}^2 u = \gamma\xi,$$

with the effective oscillation frequency

$$\omega_{eff} = 2\omega_1 \sqrt{\frac{S\omega_3}{\omega_2}}.$$

However, for very small $\zeta \to 0$ the life is more complicated. Let us put $\zeta = 0$ in Eqs.(23) and (24). Keeping in mind that $\gamma \ll \omega_1$, we may write the solutions as the sums

$$x = x_1 + x_2, \qquad z = z_1 + z_2. \tag{25}$$

The equations for the functions x_1 and z_1 are

$$\frac{d^2 x_1}{dt^2} + S\omega_1^2 z_1 x_1 = 0 \tag{26}$$

and, respectively,

$$\frac{d^2 z_1}{dt^2} + 8S\omega_1^2 z_1^2 = 0. \tag{27}$$

The corresponding initial conditions are

$$x_1(0) = x_0, \qquad \dot{x}_1(0) = v_0^x,$$

$$z_1(0) = z_0, \qquad \dot{z}_1(0) = v_0^z. \tag{28}$$

The functions x_2 and z_2 are due to the existence of random collisions and satisfy the equations

$$\frac{d^2 x_2}{dt^2} + S\omega_1^2 (z_1 x_2 + x_1 z_2) = \gamma\xi \tag{29}$$

and, respectively,

$$\frac{d^2 z_2}{dt^2} + 16S\omega_1^2 z_1 z_2 = \gamma\xi. \tag{30}$$

The related initial conditions are

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

$$z_2(0) = 0, \qquad \dot{z}_2(0) = 0. \tag{31}$$

The procedure of handling Eqs.(26), (27), (29), and (30) is as follows. First, we solve Eq.(27) whose exact solution is

$$z_1(t) = -\frac{3}{4S\omega_1^2}\mathcal{P}(t - t_0), \tag{32}$$

where $\mathcal{P}(t)$ is the Weierstrass function with the delay time

$$t_0 = \tau_0 \int_{-\infty}^{z_0} \frac{dz}{\sqrt{z_m^3 - z^3}}, \tag{33}$$

in which

$$\tau_0 \equiv \sqrt{\frac{3}{16S\omega_1^2}}, \tag{34}$$

the spin S is assumed to be positive, and

$$z_m^3 = z_0^3 + (v_0^z \tau_0)^2. \tag{35}$$

Then, the solution (32) is substituted into Eq.(26) yielding the Lamé equation of degree $1/2$. The exact solution of the latter is

$$x_1(t) = \left[c_1 \mathcal{P}\left(\frac{t - t_0}{2}\right) + c_2\right] E_3^{-1/2}\left(\frac{t - t_0}{2}\right), \tag{36}$$

with $E_3(t) \equiv d\mathcal{P}(t)/dt$ being a Lamé function of degree 3, of the first kind, and with c_1 and c_2 being integration constants.

Solving Eqs.(29) and (30), the functions x_2 and z_2, due to random collisions, can be treated as fast, as compared to x_1 and z_1. The stochastic variable ξ is modelled by the white Gaussian noise with the stochastic averages

$$\langle\langle \xi(t) \rangle\rangle = 0, \qquad \langle\langle \xi(t)\xi(t') \rangle\rangle = 2D\delta(t - t'), \tag{37}$$

where D is a diffusion rate.

From Eq.(30) we have

$$z_2(t) = \int_0^t G_z(t - \tau)\gamma\xi(\tau)d\tau \tag{38}$$

and from (29) we find

$$x_2(t) = \int_0^t G_x(t - \tau)[\gamma\xi(\tau) - S\omega_1^2 x_1 z_2(\tau)]d\tau, \tag{39}$$

the transfer functions being

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

with the effective frequency

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

The realization of stochastic averaging is based on (37), which gives

$$\langle\langle x_2(t) \rangle\rangle = 0, \qquad \langle\langle z_2(t) \rangle\rangle = 0. \tag{40}$$

For the mean–square deviation of the axial variable, Eq.(38) yields

$$\langle\langle z_2^2(t)\rangle\rangle = \frac{\gamma^2 Dt}{16\varepsilon^2}\left[1 - \frac{\sin(8\varepsilon t)}{8\varepsilon t}\right]. \tag{41}$$

Using (41) in (39), we obtain the mean–square deviation for the radial variable

$$\langle\langle x_2^2(t)\rangle\rangle = \frac{\gamma^2 Dt}{\varepsilon^2}\left[1 - \frac{\sin(2\varepsilon t)}{2\varepsilon t}\right] +$$

$$+\frac{\gamma^2 Dt x_1^2}{3600\varepsilon^2 z_1^2}\left\{1 - \cos(\varepsilon t)\cos(4\varepsilon t) + \frac{\sin(4\varepsilon t)}{4\varepsilon t}\left[\cos(\varepsilon t) - \cos(4\varepsilon t) - 16\varepsilon t\sin(\varepsilon t)\right]\right\}. \tag{42}$$

To analyze the behaviour of the found solutions, take, for concreteness, $S > 0$. For the negative S , the situation is symmetrical. Then Eq.(32) shows that z_1 is bounded from above by the maximal value (35) and diverges to $-\infty$ as $t \to t_0$ by the law

$$z_1(t) \propto -|t - t_0|^{-2}. \tag{43}$$

Such a motion, confined from one side of the z –axis and deconfined from another side, can be called *semi–confined.*

The radial variable in (36) diverges together with the axial one following the law

$$x_1(t) \propto |t - t_0|^{-1/2}. \tag{44}$$

The axial divergence is much faster than the radial one, so that the aspect ratio

$$\left[\frac{x_1^2(t)}{z_1^2(t)}\right]^{1/2} \propto |t - t_0|^{3/2} \tag{45}$$

tends to zero, as $t \to t_0$. Thus, the atomic cloud would acquire the ellipsoidal shape stretched in the axial direction.

For the random variable z_2 , Eq.(41) gives

$$\langle\langle z_2^2(t)\rangle\rangle \propto |t - t_0|^3 \exp\left(4\sqrt{3}\frac{t}{|t - t_0|}\right), \tag{46}$$

as $t \to t_0$. And from Eq.(42) we get

$$\langle\langle x_2^2(t)\rangle\rangle \propto |t - t_0|^6 \exp\left(4\sqrt{3}\frac{t}{|t - t_0|}\right). \tag{47}$$

The aspect ratio for the random variables,

$$\left[\frac{\langle\langle x_2^2(t)\rangle\rangle}{\langle\langle z_2^2(t)\rangle\rangle}\right]^{1/2} \propto |t - t_0|^3, \tag{48}$$

also tends to zero, as $t \to t_0$. However, this anisotropy is due to the preexponential factors, while the values (46) and (47) diverge by the same exponential law, that is the divergence is practically isotropic.

What kind of regime establishes in a trap, either isotropic exponential expansion or anisotropic semi–confined motion, depends on 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 small, and the atomic motion is characterized by the regular terms x_1 and z_1 . In the opposite case, when $\gamma^2 D \gg \omega_1^3$, the motion is governed by the random terms. The crossover point between these regimes is defined by the equality

$$\gamma^2 D = \omega_1^3. \tag{49}$$

Assuming that the diffusion rate $D \approx k_B T/\hbar$ we obtain from (49) the crossover temperature

$$T_c = \frac{\hbar\omega_1^3}{k_B\gamma^2}. \tag{50}$$

For the parameters typical of experiments[21,22], Eq.(50) gives $T_c \sim 10^{-7}K$.

V. Conclusion

Dynamics of neutral atoms in quadrupole magnetic traps is analysed by solving the evolution equations with the help of the method of scale separation[3-5]. This method is more general than the adiabatic approximation and, thus, permits to explore nonadiabatic regimes of atomic motion. A new semi–confined regime of motion is discovered, when atoms are confined from one side of the trap but are not confined from another. During this regime, occurring at low temperatures, the cloud of atoms acquires ellipsoidal shape stretched in the axial direction and moving to one side of the z – axis.

The semi–confining regime can be exploited for studying the relative motion of one atomic component through another. The possibility of the simultaneous trapping of two different atomic species, sodium and potassium, has been recently reported[23]. The relative motion can be achieved if one of the components is confined while another is semi–confined. A variety of unusual phenomena can happen in mixtures with relative motion. For example, in such a binary mixture the effect of conical stratification[24] can occur. Another plausible application of the semi–confining regime is for atom lasers that are being discussed in literature[25]. One of the necessary conditions for the effective operation of such a laser is the directed motion of atoms. The semi–confining regime, providing the directed atomic motion, can serve as a dynamical mechanism for the atom laser.

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