Effect of micromotion on the distribution function of ions cooled by laser light in a radiofrequency trap

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A time-dependent distribution function is derived for an ion which is cooled by laser light in a trap with an oscillating potential.

High-precision measurements of the frequency positions of the centers of transition lines of ions, which are cooled in radiofrequency (Paul) traps, raise the hope for their applications as rf and optical clocks (Ref. 1, for example). These applications stiffen the requirements on the accuracy with which the motion of the ions in the trap is described. All the existing theoretical results have been derived through the use of a pseudopotential.[2,3] That approach makes it impossible to describe the effect of micromotion on the ion distribution in a trap. It makes it also impossible to evaluate the distortions in the ion absorption spectrum which stem from this motion.

In this letter we offer an exact solution of the Fokker–Planck equation for the coordinate–velocity distribution function $\rho(x,v,t)$ of an ion being cooled in a Paul trap:

$$\frac{\partial\rho}{\partial t}+v\frac{\partial\rho}{\partial x}+\frac{F}{m}\frac{\partial\rho}{\partial v}=\beta\frac{\partial}{\partial v}(v\rho)+D\Delta_v\rho, \tag{1}$$

$$F=m[a+b\cos(\Omega t)]x.$$

Here F is the force acting on an ion in the trap (this force oscillates in time), and m is the mass of the ion. The right side of (1) describes the effect of the cooling laser field, $m\beta v$ is the friction force, and D is the diffusion coefficient in velocity space.[2,4,5] To simplify the discussion we will use a 1D equation; the generalization to the 3D case is obvious.

Following Ref. 5, we transform from (1) to an equation for the Fourier transform of the distribution function:

$$\frac{\partial f}{\partial t}-\eta\frac{\partial f}{\partial\xi}-[a+b\cos(\Omega t)]\xi\frac{\partial f}{\partial\eta}+\beta\xi\frac{\partial f}{\partial\xi}=-D\xi^2 f, \tag{2}$$

$$f(\xi,\eta,t)=\int\exp(iv\xi+i\eta x)\rho(x,v,t)dxdv.$$

Along the trajectory defined by the equations

$$\dot{\xi}=-\eta+\beta\xi,\quad \dot{\eta}=-[a+b\cos(\Omega t)]\xi, \tag{3}$$

the left side of (2) is a total time derivative, $df/dt=-D\xi^2(t)f$. We can thus write

$$f(t)=f_0(\xi_0,\eta_0)\,\exp\left(-D\int_0^t \xi^2(t)dt\right), \tag{4}$$

where $f_0(\xi,\eta)$ is the Fourier transform of the distribution function at $t=0$, and ξ_0 and η_0 are the coordinates of the trajectory at $t=0$.

From Eqs. (3) we have

$$\ddot{\xi}-\beta\dot{\xi}-[a+b\,\cos(\Omega t)]\xi=0. \tag{5}$$

For the function $\chi=\exp(-\beta t/2)\xi(t)$ we find the Mathieu equation[6]

$$\ddot{\chi}+[A-B\cos^2(\Omega t/2)]\chi=0, \tag{6}$$

$$A=b-a-\beta^2/4,\quad B=2b.$$

A general solution of that equation is

$$\chi=Ce^{i\omega t}\sum_{n=-\infty}^{\infty} a_n e^{in\Omega t}+C^*e^{-i\omega t}\sum_{n=-\infty}^{\infty} a_n^* e^{-in\Omega t}, \tag{7}$$

where C is an arbitrary constant.

A procedure was worked out in Ref. 6 for finding the frequency of the secular motion, ω, and the coefficients a_n. That search can be carried out with any prespecified accuracy. Solely to simplify the problem, we make use of the circumstance that the conditions $\beta\ll\omega\ll\Omega$ and $|a_1|$, $|a_{-1}|\ll|a_0|$ hold in the traps ordinarily used. From (3), (6), and (7) we find the following expressions, within terms on the order of ω/Ω, inclusively:

$$\xi=e^{\beta t/2}(Ce^{i\omega t}+C^*e^{-i\omega t})[1+\alpha\cos(\Omega t)],$$

$$\eta=e^{\beta t/2}\{Ce^{i\omega t}[-i\omega+\alpha\Omega\sin(\Omega t)]$$

$$+C^*e^{-i\omega t}[i\omega+\alpha\Omega\,\sin(\Omega t)]\}, \tag{8}$$

$$\alpha=-b/\Omega^2,\quad \omega^2=\alpha^2\Omega^2/2-a,\quad |\alpha|\ll 1,\quad |a|\ll\Omega^2.$$

We now need to carry out the time integration in (4). Ignoring the oscillating terms, which make only a small contribution, we find

$$f(\xi,\eta,t)=f_0(\xi_0,\eta_0)\exp\left(-\frac{D\cdot 2|C|^2}{\beta}[e^{\beta t}-1]\right), \tag{9}$$

$$\xi_0=C+C^*,\quad \eta_0=i\omega C+i\omega C^*.$$

To find the final result, we can express the quantities C and C^* in Eq. (9) in terms of the instantaneous values of ξ and η, making use of Eq. (8):

$$C=1/2[\xi+i\eta/\omega-iq\xi\,\sin(\Omega t)]e^{-\beta t/2-i\omega t},\quad q=\alpha\Omega/\omega. \tag{10}$$

Equations (9) and (10) give us the Fourier transform of the time-dependent ion distribution function in a Paul trap for an arbitrary initial distribution function. For large time intervals $t\gg 1/\beta$, this function becomes independent of the initial conditions [the normalization condition gives us $f_0(\xi=0,\eta=0)=1$] and takes the form

$$f_\infty(\xi,\eta,t)\exp\left\{-\frac{D}{2\beta}\left[\xi^2+\frac{\eta^2}{\omega^2}-2q\xi\frac{\eta}{\omega}\ \sin(\Omega t)+q^2\xi^2\sin^2(\Omega t)\right]\right\} \tag{11}$$

or, in terms of the customary coordinates,

$$\rho_\infty(v,x,t)=\frac{\beta\omega}{2\pi D}\exp\left(-\frac{\beta}{2D}\{x^2\omega^2[1+q^2\sin^2(\Omega t)]+v^2+2xvq\sin(\Omega t)\}\right). \tag{12}$$

The coefficient $2D/\beta$ depends on the particular cooling scheme. Under optimum conditions it is[2,3,5,7] $2D/\beta\sim\hbar\Gamma$ in order of magnitude, where Γ is the radiative linewidth of the transition used for cooling.

If the initial distribution function is a δ-function $\rho_0(x,v)=\delta(x-x_0)\delta(v-v_0)$, which corresponds to $f_0(\xi,\eta)=\exp(iv_0\xi+ix_0\eta)$, then the inverse Fourier transform of (9) can be found analytically. The resulting Green's function is

$$\rho(x,v;x_0,v_0,t)=\frac{\omega}{\pi}S\ \exp[-S\varphi(x,v,t)], \tag{13}$$

$$\varphi(x,v,t)=[\omega x-[\omega x_0\cos(\omega t)+v_0\sin(\omega t)]e^{-\beta t/2}]^2$$
$$+\{v+\omega xq\sin(\Omega t)-[v_0\cos(\omega t)-x_0\omega\sin(\omega t)]e^{-\beta t/2}\}^2,$$

$$S=\frac{\beta}{2D}(1-e^{-\beta t})^{-1}.$$

Under the condition $\beta t\gg 1$ this function is the same as (12).

It can be seen from (12) that the limiting distribution function is not a Maxwell–Boltzmann distribution, and to introduce the concept of a temperature is generally not legitimate. Integrating (12) over the coordinate, we find

$$G(v,t)=\int\rho_\infty(v,x,t)dx=\left(\frac{\beta}{2\pi D[1+q^2\sin^2(\Omega t)]}\right)^{1/2}\exp\left(-\frac{\beta}{2D}\frac{v^2}{1+q^2\sin^2(\Omega t)}\right).$$

This expression has the form of a Maxwellian distribution with a time-modulated temperature $k_BT=(mD/\beta)[1+q^2\sin^2(\Omega t)]$. The mean temperature is $k_B\bar{T}=(mD/\beta)\times(1+q^2/2)$; here $(q^2/2)(1+q^2/2)^{-1}$ is the fraction of the energy associated with the micromotion.

The 3D potential of the trap is $\Phi=[U+V\cos(\Omega t)](x^2+y^2-2z^2)$; i.e., the quantities a_i and b_i are related by $a_x=a_y=-a_z/2=a_0$, $b_x=b_y=-b_z/2=b_0$. The fraction of the energy of the micromotion in the 3D case is therefore $(2-L-2L^2)^{-1}$, where $L=a_0\Omega^2/b_0^2$. We thus see that half of the total energy is in the micromotion in two cases:[7] the case $L=0$ (there is no static potential; $\omega_x=\omega_y=\omega_z/2$) and the case $L=-1/2$ ($\omega_x=\omega_y=\omega_z$). It can be seen from (8) that the condition for stability of the trap ($\omega_i^2>0$) is $-1<L<1/2$.

Using the relation $m<v_i^2>/2=k_B\bar{T}_i$, we can calculate the frequency shift Δ due to the second-order Doppler effect which is a quantity of importance for a frequency standard:

$$\Delta = -\frac{1}{2}\omega_0\frac{\langle v^2\rangle}{c^2} = -\omega_0\frac{3D}{\beta c^2}\left(1+\frac{1}{1-L-2L^2}\right).$$

Here ω_0 is the frequency of the resonant molecular transition. This quantity increases as the stability boundaries are approached. The minimum value of Δ is reached in the case $L=-1/4$, which corresponds to $\omega_x^2=\omega_y^2=\omega_z^2/2$.

Collisions with the surrounding gas may have an important effect on the ion distribution function and on the limiting temperature. If we use the weak-collision model[5,8] to describe this effect, we find that solutions (9) and (12), and also Green's function (13), remain the same in form upon the substitution $\beta\rightarrow\beta+\mu$ and $D\rightarrow D+\mu v_0^2/2$, where μ is the collision rate, and v_0^2 is the mean square velocity of the gas molecules. Using the Green's function or, more precisely, its Fourier transform (9), we can calculate the correlation function[8] and solve the problem of how the micromotion and collisions affect the shape of the absorption line of an ion being cooled in the trap. Such calculations require stating more clearly the conditions under which the measurements were carried out. These calculations will be carried out in a more-detailed publication.

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[1] M. G. Raizen *et al.*, J. Mod. Opt. **39**, 233 (1992).
[2] S. Stenholm, Rev. Mod. Phys. **58**, 699 (1986).
[3] P. E. Toschek, Usp. Fiz. Nauk **158**, 451 (1989).
[4] V. G. Minogin and V. S. Letokhov, *Laser Light Pressure on Atoms* (Gordon and Breach, New York, 1987).
[5] V. A. Alekseev and D. D. Krylova, J. Opt. Soc. Am. B **10**, 1545 (1993).
[6] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 1, §5.2.
[7] D. J. Wineland *et al.*, Phys. Rev. A **36**, 2220 (1987).
[8] V. A. Alekseev *et al.*, Opt. Commun. **106**, 100 (1994).

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