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Computed energy and spatial statistical properties of stored ions cooled by a buffer gas

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We describe a three-dimensional model, based on the temporal invariance of the statistical properties, which allows us to calculate the spatial and energy probability densities of strongly confined ions in the presence of a buffer gas. This model is then applied to a population of Cs^+ ions for which we compute these densities within the whole stability diagram and for various gases. In the case of helium, in particular, we show that these laws can be described by Gaussian functions, and we present the evolution of the temporal average of the spatial dispersions and ionic temperatures at the working point.

I. INTRODUCTION

Ion storage by rf quadrupole field trapping is a particularly efficient research tool in atomic physics.[1,2] Indeed, it is possible to maintain an ionic population for long periods of time (from a few seconds to several hours) free from magnetic fields, collisions, and walls effects. Moreover, because of the quasiperiodic movement of the ions in each direction, the first-order Doppler effect is discrete.[3] The second-order Doppler effect can be reduced by such techniques as radiative,[4,5] collisional,[6-9] and optical cooling.[10-12] Then the equilibrium state of the trapped ions is close to the thermodynamic equilibrium. These properties allow one to study long-lived phenomena[7,9,13] (e.g., lifetimes of metastable states and autodetachement processes)[14,15] and spectroscopy at very high resolution (e.g., hyperfine structure and frequency standards).[16-19]

To this end it is useful to know the energy and spatial properties of the ionic populations. We have previously established[20,21] a stochastic model which permits us to describe such statistical behaviors as the lifetime of the ions and the energy and spatial distributions in the presence of infrequent elastic collisions with a neutral atomic gas. In particular, we have shown that the introduction of a light gas can increase the lifetime and reduce the mean values of the energetic properties of the ions. Moreover, we have shown that these distributions tend to Gaussian distributions after some initial reorganization time. The application of this formalism, however, does not allow one to treat, in a general manner, the three-dimensional case because it would require excessive computer time and memory, and we have used an approximate method in a previous study.[22] Following this work we introduced an easier method, based on the temporal invariance of the statistical properties due to the periodicity of the rf field, which allows us to verify the assumed form of the distribution and to compute their parameters. It has been successfully tested for the one-dimensional (1D) case[23] and its use on a realistic three-dimensional (3D) model has turned out to be interesting in the study of space-charge effects.[24]

In this paper, we apply this method to obtain the parameters which describe the energy and spatial distributions and show the limits of the validity of a Gaussian pattern. Firstly, we present the principle of the method applied to a 3D model, after which we explain the criterion chosen to decide whether or not the distributions may be represented by a Gaussian function and finally we show the results obtained from a systematic study of the stability diagram.

The present study concerns positive cesium ions in a radio-frequency field of period $\Omega/2\pi = 10^6/2\pi$ rad s^{-1}. Nevertheless, results are valid for values of Ω which can be in a large range around this one. The ions evolve in a trap of large dimension with a dilute buffer gas (conditions which are always satisfied with collisional cooling). The partial pressure of the buffer gas does not exceed 10^{-4} mm. Under these conditions, the time between ion-atom collisions is approximately equal to 100 periods of the radio-frequency field. Space-charge phenomena are neglected here. These hypotheses are realistic when the total number of ions is not greater than 10^4.[25] In this case, the mean time between two ion-ion collisions is of the order of several seconds and heating which could occur because of the inhomogeneity of the rf field cannot be induced.

II. FORMALISM (REF. 22)

The dynamic state $(\vec{x},\dot{\vec{x}})$ of each ion cannot be known but can be described by a random process $(\vec{X}(t),\dot{\vec{X}}(t))$ whose properties are Markovian because of the shortness of the interaction time compared with the other characteristic times. After some collisions, the initial conditions are forgotten and $(\vec{X}(t),\dot{\vec{X}}(t))$ reaches an asymptotic regime. The associated probability law, rigorously depends on the confinement well depth, but when this is increased (while staying within the values generally used experimentally), the probability law rapidly converges to a limit independent of the depth. Therefore one can replace the real trap by one of infinite depth. The function $(\vec{X}(t),\dot{\vec{X}}(t))$ associated with the asymptotic behavior and defined by the probability density $f_{X\dot{X}}(\vec{x},\dot{\vec{x}},t)$ is not stationary because of the periodicity of the radio-frequency field. It is, however, invariant to any temporal translation of the driving field which is a multiple of $T_m=2\pi/\Omega$.

Thus, setting g, an arbitrary function of $(\vec{x},\dot{\vec{x}})$, and setting

$$G(t)=g(\vec{X}(t),\dot{\vec{X}}(t))\ ,$$

to be the corresponding random function. $G(t)$ is also invariant, for any sequence of times

$$t_0, t_1=t_0+T_m, \ldots, t_j=t_0+jT_m\ .$$

The mean values $\langle G(t_0)\rangle$, $\langle G(t_1)\rangle, \ldots,$ $\langle G(t_j)\rangle$ are equal.

This property permits us to establish a relation which must be satisfied for any function G when $f_{X\dot{X}}(\vec{x},\dot{\vec{x}},t)$ is suitable. $\langle G(t_0)\rangle$ is simply written as

$$\langle G(t_0)\rangle=\int g(\vec{x},\dot{\vec{x}})f_{X\dot{X}}(\vec{x},\dot{\vec{x}},t)d\vec{x}\,d\dot{\vec{x}}\ . \tag{2.1}$$

Let k be a particular value of j. In order to calculate $\langle G(t_k)\rangle$ we must take account of the different events which occur between t_0 and t_k. These events depend on ρ_2, the bulk density of the gas atoms, $f_{V_2}(\vec{v}_2)$, the probability density of the velocity of this gas, and s, the ion-atom collision cross section. Because ρ_2 is small, the probability that more than one collision occurs between t_0 and t_k, which can be chosen here, is negligible, providing one limits the maximum value of k. Let $f_C(\vec{c})$ be the two parameter function which describes the collision. In the absence of collisions between two instants t and t', we let $\mathscr{L}_{t\to t'}$ be the determinist function which allows one to obtain $(\vec{x}(t'),\dot{\vec{x}}(t'))$ from $(\vec{x}(t),\dot{\vec{x}}(t))$.

The mean value $\langle G(t_k)\rangle$ depends on the history of the ion between t_0 and t_k:

(i) If $(\vec{x}(t_0),\dot{\vec{x}}(t_0))=(\vec{x}_0,\dot{\vec{x}}_0)$ is known and if no collision occurs between t_0 and t_k with probability

$$1-\rho_2 s\int_{t_0}^{t_0+kT_m}\int f_{V_2}(\vec{v}_2)\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\,d\vec{v}_2dt\ ,$$

then $G(t_k)=g(\vec{x}_k,\dot{\vec{x}}_k)$, where

$$(\vec{x}_k,\dot{\vec{x}}_k)=\mathscr{L}_{t_0\to t_k}(\vec{x}_0,\dot{\vec{x}}_0)\ .$$

(ii) If $(\vec{x}(t_0),\dot{\vec{x}}(t_0))$ is known and if one collision occurs between t and $t+dt$, $t_0<t<t_k$, with the incident atom having a velocity between $\vec{v}_2$ and $\vec{v}_2+d\vec{v}_2$ and collision parameters between $\vec{c}$ and $\vec{c}+d\vec{c}$, with probability

$$\rho_2 s\, f_{V_2}(\vec{v}_2)f_C(\vec{c})\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\,d\vec{v}_2d\vec{c}\;dt\ ,$$

then $G(t_k)=g(\vec{x}\,'_k,\dot{\vec{x}}\,'_k)$, where $(\vec{x}\,'_k,\dot{\vec{x}}\,'_k)$ is obtained from $(\vec{x}\,'(t),\dot{\vec{x}}\,'(t))$ by $(\vec{x}\,'_k,\dot{\vec{x}}\,'_k)=\mathscr{L}_{t\to t_k}(\vec{x}\,'(t),\dot{\vec{x}}\,'(t))$. Here $(\vec{x}\,'(t),\dot{\vec{x}}\,'(t))$ is the new dynamical state, acquired at the instant t due to the collision, obtained from the calculation of

$$(\vec{x}(t),\dot{\vec{x}}(t))=\mathscr{L}_{t_0\to t_k}(\vec{x}_0,\dot{\vec{x}}_0)\ .$$

(iii) Without information on $(\vec{x}_0,\dot{\vec{x}}_0)$, $\vec{v}_2$, and $\vec{c}$, and on the instant t of the collision (or its existence), the mean value of $G(t_k)$ is obtained by weighting the results obtained in (i) and (ii) by the probability of their realization. Let $f_{X_0\dot{X}_0}(\vec{x}_0,\dot{\vec{x}}_0)$ be the value of $f_{X\dot{X}}(\vec{x},\dot{\vec{x}},t_0)$; then

$$\langle G(t_k)\rangle=\int g(\vec{x}_k,\dot{\vec{x}}_k)\left[1-\rho_2 s\int_{t_0}^{t_0+kT_m}\left[\int f_{V_2}(\vec{v}_2)\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\,d\vec{v}_2\right]dt\right]f_{X_0\dot{X}_0}(\vec{x}_0,\dot{\vec{x}}_0)d\vec{x}_0\,d\dot{\vec{x}}_0$$

$$+\int_{t_0}^{t_0+kT_m}\left[\int f_{X_0\dot{X}_0}(\vec{x}_0,\dot{\vec{x}}_0)\int \rho_2 s f_{V_2}(\vec{v}_2)\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\int f_C(\vec{c}\,)g(\vec{x}\,'_k,\dot{\vec{x}}\,'_k)d\vec{x}_0\,d\dot{\vec{x}}_0\,d\vec{v}_2\,d\vec{c}\,\right]dt\ ,$$

but $\langle G(t_k)\rangle=\langle G(t_0)\rangle$. So,

$$\rho_2 s\int_{t_0}^{t_0+kT_m}\left[\int f_{X_0\dot{X}_0}(\vec{x}_0,\dot{\vec{x}}_0)\int f_{V_2}(\vec{v}_2)\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\,[f_C(\vec{c}\,)g(\vec{x}\,'_k,\dot{\vec{x}}\,'_k)d\vec{c}-g(\vec{x}_k,\dot{\vec{x}}_k)]d\vec{x}_0\,d\dot{\vec{x}}_0\,d\vec{v}_2\right]dt$$
$$-\int[g(\vec{x}_0,\dot{\vec{x}}_0)-g(\vec{x}_k,\dot{\vec{x}}_k)]f_{X_0\dot{X}_0}(\vec{x}_0,\dot{\vec{x}}_0)d\vec{x}_0 d\dot{\vec{x}}_0=0\ . \quad (2.2)$$

Let $I(g,f_{X_0\dot{X}_0})$ be the left-hand side of (2.2); $I(g,f_{X_0\dot{X}_0})$ can be used to determine $f_{X_0\dot{X}_0}$: the method consists of finding the function h of $\vec{x}_0$ and $\dot{\vec{x}}_0$ for which $I(g,h)$ equals zero for any function g. In fact, the problem is difficult to solve in the general case but can by simplified for small values of ρ_2.

$f_{X_0\dot{X}_0}$ depends on $\rho_2 s$ and it is possible to make an expansion over successive powers of $\rho_2 s$ by setting

$$f_{X_0\dot{X}_0}(\vec{x},\dot{\vec{x}})=f_0(\vec{x},\dot{\vec{x}})+\rho_2 s f_1(\vec{x},\dot{\vec{x}})$$
$$+(\rho_2 s)^2 f_2(\vec{x},\dot{\vec{x}})+\cdots \quad (2.3)$$

and imposing the restriction that $f_0(\vec{x},\dot{\vec{x}})$ be normed. Thus $f_0(\vec{x}_0,\dot{\vec{x}}_0)$ also represents a probability density. $f_{X_0\dot{X}_0}$ looks like a “smooth density” function f_0 on which a fine structure (the other terms of the expansion) is superposed. The importance of these terms are negligible here because of the supposed value of $\rho_2 s$.

The fundamental information about $f_{X_0\dot{X}_0}$ is therefore given by f_0 which we, now, seek to determine. Setting (2.3) in (2.2), $I(g,f_{X_0\dot{X}_0})$ is identically zero if all the coefficients associated with the successive powers of $\rho_2 s$ are zero, from which a hierarchical system of equations can be inferred.

The first equation of this system [associated with $(\rho_2 s)^0$] can be written

$$\int[g(\vec{x}_0,\dot{\vec{x}}_0)-g(\vec{x}_k,\dot{\vec{x}}_k)]f_0(\vec{x}_0,\dot{\vec{x}}_0)d\vec{x}_0 d\dot{\vec{x}}_0=0\ . \quad (2.4)$$

The second equation, where the influence of collisions appears, is

$$\int_{t_0}^{t_0+kT_m}\left[\int f_0(\vec{x}_0,\dot{\vec{x}}_0)\int f_{V_2}(\vec{v}_2)\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\left[\int f_C(\vec{c}\,)g(\vec{x}'_k,\dot{\vec{x}}\,'_k)d\vec{c}-g(\vec{x}_k,\dot{\vec{x}}_k)\right]d\vec{x}_0\,d\dot{\vec{x}}_0\,d\vec{v}_2\right]dt$$
$$=\int[g(\vec{x}_0,\dot{\vec{x}}_0)-g(\vec{x}_k,\dot{\vec{x}}_k)]f_1(\vec{x}_0,\dot{\vec{x}}_0)d\vec{x}_0\,d\dot{\vec{x}}_0\ . \quad (2.5)$$

Equation (2.5) includes two unknown functions f_0 and f_1. f_1 can be eliminated in the following way: Think of some properties of the motion of the ion in the trap.[1] Let $\xi(t),\dot{\xi}(t)$ ($\xi=x$, y, or z) be the components of $(\vec{x}(t),\dot{\vec{x}}(t))$. They are expressed according to the two constants of the motion (u_ξ,φ_ξ) by the relations

$$\xi(t)=\frac{u_\xi}{\omega_\xi}\{[1+A_\xi(t)]\cos(\omega_\xi t-\varphi_\xi)-B_\xi(t)\sin(\omega_\xi t-\varphi_\xi)\}\ , \quad (2.6)$$
$$\dot{\xi}(t)=-u_\xi\{C_\xi(t)\cos(\omega_\xi t-\varphi_\xi)+[1+D_\xi(t)]\sin(\omega_\xi t-\varphi_\xi)\}\ ,$$

where $A_\xi(t)$, $B_\xi(t)$, $C_\xi(t)$, $D_\xi(t)$ are trigonometric series of the successive harmonics of the driving frequency. The fundamental frequency $\omega_\xi/2\pi$ depends on the working voltage $(\omega_x=\omega_y)$. The quantities

$$\left[\frac{\omega_\xi\xi(kT_m)}{1+A_\xi(kT_m)}\right]^2+\left[\frac{\dot{\xi}(kT_m)}{1+D_\xi(kT_m)}\right]^2=u_\xi^2 \quad (2.7)$$

are invariants.

If we choose for the function g a function of $\vec{u}$, then (2.5) is simplified, and with k equal to 1 it becomes

$$\int_{t_0}^{t_0+T_m}\int f_0(\vec{x}_0,\dot{\vec{x}}_0)\int f_{V_2}(\vec{v}_2)\,|\,\vec{v}_2-\dot{\vec{x}}(t)\,|\,[f_C(\vec{c}\,)g(\vec{u}\,'_k)d\vec{c}-g(\vec{u}_k)]d\vec{x}_0\,d\dot{\vec{x}}_0\,d\vec{v}_2\,dt=0\ , \tag{2.8}$$

therefore f_0 must be a solution of this equation.

It is easy to see that f_0 does not depend on the frequency Ω of the rf field by a change of variables.

III. DETERMINATION OF f_0

The following remarks allow us to be more precise about f_0: As a result of the cylindrical symmetry of the trap, f_0 may be written

$$f_0(x_0,\dot{x}_0,y_0,\dot{y}_0,z_0,\dot{z}_0)$$
$$=\varphi((x_0^2+y_0^2)^{1/2},(\dot{x}_0^2+\dot{y}_0^2)^{1/2},z_0,\dot{z}_0)\ , \tag{3.1}$$

but we also know that (cf. the Appendix) if u_x and u_z are the invariants corresponding to $(\vec{x}_0,\dot{\vec{x}}_0)$ and $(\vec{z}_0,\dot{\vec{z}}_0)$, it follows that

$$f_0(x_0,\dot{x}_0,0,0,z_0,\dot{z}_0)=\psi(u_x,u_z)$$

and from (3.1) we have

$$f_0(x_0,\dot{x}_0,0,0,z_0,\dot{z}_0)=\varphi(\,|\,x_0\,|\,,\,|\,\dot{x}_0\,|\,,z_0,\dot{z}_0), \tag{3.2}$$

from which it can be deduced that

$$\varphi(\,|\,x_0\,|\,,\,|\,\dot{x}_0\,|\,,z_0,\dot{z}_0)=\psi(u_x,u_z)$$

and therefore that

$$\varphi((x_0^2+y_0^2)^{1/2},(\dot{x}_0^2+\dot{y}_0^2)^{1/2},z_0,\dot{z}_0)$$
$$=\psi((u_x^2+u_y^2)^{1/2},u_z)\ .$$

Consequently, we will choose functions f_0 which depend on the quantities

$$\frac{\omega_x^2(x_0^2+y_0^2)}{[1+A_x(0)]^2}+\frac{\dot{x}_0^2+\dot{y}_0^2}{[1+D_x(0)]^2}\ ,$$
$$\frac{\omega_z^2z_0^2}{[1+A_z(0)]^2}+\frac{\dot{z}_0^2}{[1+D_z(0)]^2}\ .$$

The previous works[14,16] have shown that in the case of a light buffer gas $f_{x_0\dot{x}_0}$ and thus, f_0, are close to being Gaussian; therefore, we assume, initially, a function f_0 whose form is

$$\frac{K}{8\pi^3\sigma_{0x}^4\sigma_{0z}^2}\exp\left[-\left\{\frac{\omega_x^2(x_0^2+y_0^2)}{2\sigma_{0x}^2[1+A_x(0)]^2}+\frac{\dot{x}_0^2+\dot{y}_0^2}{2\sigma_{0x}^2[1+D_x(0)]^2}+\frac{\omega_z^2z_0^2}{2\sigma_{0z}^2[1+A_z(0)]^2}+\frac{\dot{z}_0^2}{2\sigma_{0z}^2[1+D_z(0)]^2}\right]\right]\ , \tag{3.3}$$

where K is a normalization factor.

The marginal laws are expressed, in this case, for the x components, for instance, of the position and the velocity by

$$\frac{1}{\sqrt{2\pi}\ \sigma_{sx0}}\exp\left[-\frac{x_0^2}{2\sigma_{sx0}^2}\right]$$

with

$$\sigma_{sx0}=\sigma_{0x}\frac{1+A_x(0)}{\omega_x}$$

and

$$\frac{1}{\sqrt{2\pi}\ \sigma_{vx0}}\exp\left[-\frac{\dot{x}_0^2}{2\sigma_{vx0}^2}\right]$$

with

$$\sigma_{vx0}=\sigma_{0x}[1+D_x(0)]\ .$$

σ_{sx0} and σ_{vx0} characterize the distribution law at the instant t_0. Because of the invariant to translation by kT_m, we must have

$$\sigma_{sx}(kT_m)=\sigma_{sx0}$$

and

$$\sigma_{vx}(kT_m)=\sigma_{vx0}\ .$$

This is really true since $A_x(t)$ and $D_x(t)$ are periodic. Dispersions corresponding to any time are given, from (2.6), by

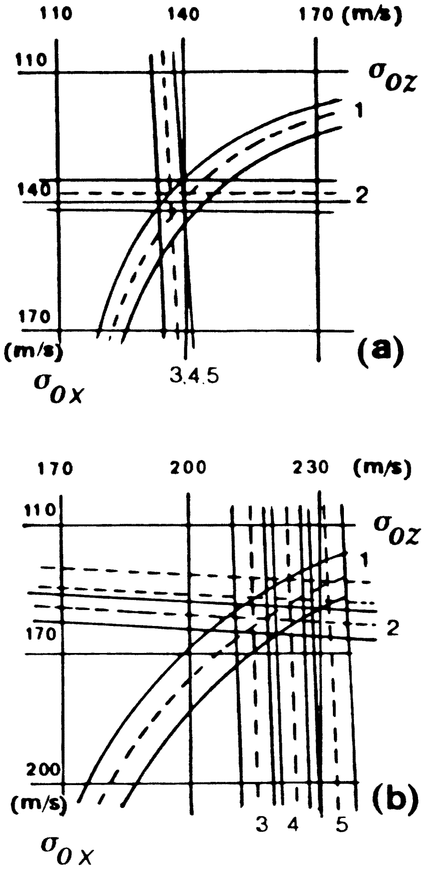

FIG. 1. Determination of the parameters σ_{0x} and σ_{0z} in the ion-distribution law (3D model) by a zero method. (a) The Gaussian model is suitable. Zeros corresponding to various functions $g(u_z)$ [and $g(u_x)$] are quasicoincident, the width of each curve indicates the uncertainty of the computation. (b) Gaussian model is not valid. Zeros of the various functions $g(u_x)$ and chiefly $g(u_z)$ are clearly separated. 1, $g(\vec{u})=u_x u_z$; 2, $g(\vec{u})=u_x$; 3, $g(\vec{u})=u_z$; 4, $g(\vec{u})=u_z^2$; 5, $g(\vec{u})=u_z^3$.

$$\sigma_{sx}(t)=\frac{\sigma_{0x}}{\omega_x}\{[1+A_x(t)]^2+B_x^2(t)\}^{1/2} \tag{3.4}$$

and

$$\sigma_{vx}(t)=\sigma_{0x}\{C_x^2(t)+[1+D_x(t)]^2\}^{1/2} . \tag{3.5}$$

From this last parameter, one deduces another parameter

$$T_x(t)=\frac{m}{k}\sigma_{0x}^2\{C_x^2(t)+[1+D_x(t)]^2\}^{1/2} , \tag{3.6}$$

where m is the mass of the ion and k the Boltzmann constant. This parameter has the same dimension as a temperature but it periodically varies very rapidly versus time. We call it the pseudotemperature of the ionic population.

The average parameters, for instance $\overline{T}_x$, can be calculated with formulas of the type

$$\overline{T}_x=\frac{1}{T_m}\int_0^{T_m} T_x(t)dt . \tag{3.7}$$

We define the temperature of the ionic population by this equation. The quantities corresponding to the direction $\vec{0z}$ are obtained by analogous formulas.

If f_0 has exactly the form given by (3.3), the problem is reduced to seeking the values σ_{0x} and σ_{0z} for which (2.8) is always zero. To this end, the integral of (2.8) is computed by substituting σ_{0x} and σ_{0z} for different values λ_x and λ_z and with various functions g. Let C_i be the curve in the (λ_x,λ_z) plane that represents the value for which (2.8) is zero corresponding to a function g_i. Then σ_{0x} and σ_{0z} are the coordinates of the intersection points of different curves, C_i. If the shape of f_0 is known, to determine these parameters it is enough to take only two functions g_i. In practice, we must verify the suitability of the functional form of f_0. To do this we must evaluate (2.8) for a larger number of functions g. We choose the following functions:

$$g_{1x}(\vec{u})=u_x,\quad g_{2x}(\vec{u})=u_x^2,\quad g_{3x}(\vec{u})=u_x^3 ,$$

$$g_{1z}(\vec{u})=u_z,\quad g_{2z}(\vec{u})=u_z^2,\quad g_{3z}(\vec{u})=u_z^3 ,$$

and

$$g_{xz}(\vec{u})=u_x u_z .$$

Let $\lambda_x^{(i)}$ and $\lambda_z^{(i)}$ be the values found for σ_{0x} and σ_{0z} for functions g_i. If f_0 is exactly Gaussian, these values are independent of i. When f_0 cannot be approximated by a Gaussian, the different pairs $(\lambda_x^{(i)},\lambda_z^{(i)})$ are distinct. Figure 1 illustrates this point. When the differences between the various pairs are of the order of the uncertainty of the result, we consider that the chosen model for f_0 is suitable. We will now explain how we can give significance to the more important divergences.

IV. CONTROL OF THE SUITABILITY OF THE PATTERN REPRESENTATION

When the form chosen for f_0 is not convenient, all the curves C_i are not concurrent. Then we must use a pattern which allows a more precise description of the probability density. To this end, it is necessary to increase the number of parameters which characterize f_0 (two in the Gaussian case) to

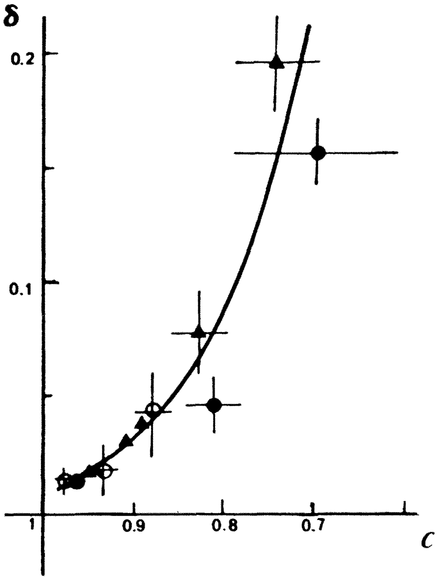

FIG. 2. Evolution of the relative spreading between the various estimates of b_i^1: δ obtained by the one-parameter method vs c. One can see that the magnitude of δ indicates the difference between the real distribution and the Gaussian one. Real distribution is chosen in the form of $K\exp(-u_z^{2c}/2b^2)$. Open circles correspond to axis $a=0$, squares at $\beta_z=0.2$, closed circles to $a=0$, $q=0.2$ and various buffer gas. (For clarity, uncertainties of the points are not always shown.)

at least four. The working of the relation (2.8) becomes more difficult. Since the aim here is essentialy qualitative, we limit this study to an 1D model ($\vec{O}z$ direction). We choose a test function which depends on two parameters:

$$K\exp\left\{-\frac{1}{2b^2}\left[\left[\frac{\omega_z z_0}{1+A_z(0)}\right]^2+\left[\frac{\dot{z}_0}{1+D_z(0)}\right]^2\right]\right\},$$

where K is the normalization factor.

When the component of f_0 in the direction $\vec{O}z$ is Gaussian, c is equal to 1 and b represents the standard deviation $\mathscr{s}$. For any other value of c, $\mathscr{s}$ is then given by

$$\mathscr{s}=bA(c)$$

when

$$A^2(c)=\frac{\int y^2\exp[-\tfrac{1}{2}(x^2+y^2)^c]dx\,dy}{\int\exp\{[-\tfrac{1}{2}(x^2+y^2)]^c\}dx\,dy}\ .$$

$A(c)$ is evaluated numerically. It is a decreasing function which is found to be between 1 and 4 for c within the range 1 to 0.5. b and c must make the expression (2.8) zero for any function g and they are looked for by a method which approaches the one described above. We use the following g functions:

$$g_1(\vec{u})=u_z;\quad g_2(\vec{u})=u_z^2;\quad g_3(\vec{u})=u_z^3\ .$$

Two of these functions are sufficient to determine the pair (b,c) which characterizes the distribution, the third is needed to check the suitability of the representation as before. For c equal to 1, the values b_i^1 of b for which (2.8) is equal to zero correspond to the various estimates of the standard deviation of a Gaussian law obtained for each function g_i. We computed the values of b, c, and b_i^1 [(2.8) is evaluated by a Monte Carlo technique], along the axis $a=0$, along the isobeta $\beta_z=0.2$ (with $\beta_x\leq 0.5$) and at the point $a=0$, $q=0.2$ for several buffer gases. In Fig. 2 we show the pairs

$$(\delta=(b_3^1-b_1^1)/b_{\text{av}}^1,c)\ ,$$

where b_{av}^1 is the arithmetic average of (b_i^1) which corresponds to each case. Practically all the points are situated on a curve and it can be seen that it is possible to associate with the spread of the values obtained by the one-parameter method a value of c which indicates the difference between the real distribution and the Gaussian distribution.

The calculations of s show that we always get $b_1^1\leq b_2^1\leq b_3^1$ and often $b_1^1\leq\mathscr{s}\leq b_2^1$. The ratios $|b_{\text{av}}^1-\mathscr{s}|/b_{\text{av}}^1$ are, in the case of helium, for any working point, always near to 1%; under these conditions, even if a Gaussian law does not represent accurately the real distribution ($0.9\geq c\geq 0.75$), the values of b_i^1 are convenient estimates of the standard deviation. For argon and krypton, for which c is close to 0.7 and 0.3, respectively, the standard deviation and b_{av}^1 differ by only 10%. We note that similar calculations[23] done in a less systematic way allowed us to foresee these results.

Finally, when c lies between 1 and 0.9, considering the lack of accuracy, the Gaussian approximate is entirely justified. For $0.9\geq c\geq 0.8$, the spacings between the various estimates are lower than 10%, we assume that the choice of a Gaussian distribution does not induce too much error and, in accordance to the uncertainty, the moment of second order is well approximated by b_1^1. Given that the spreading of the values has the same magnitude in the 3D model, we take as a criterion of the limit of the suitability of a Gaussian pattern that differences between b_i^1 are of the order of 10%.

V. RESULTS

We apply the method just described, which uses a 3D model, to an ionic population of cesium. The

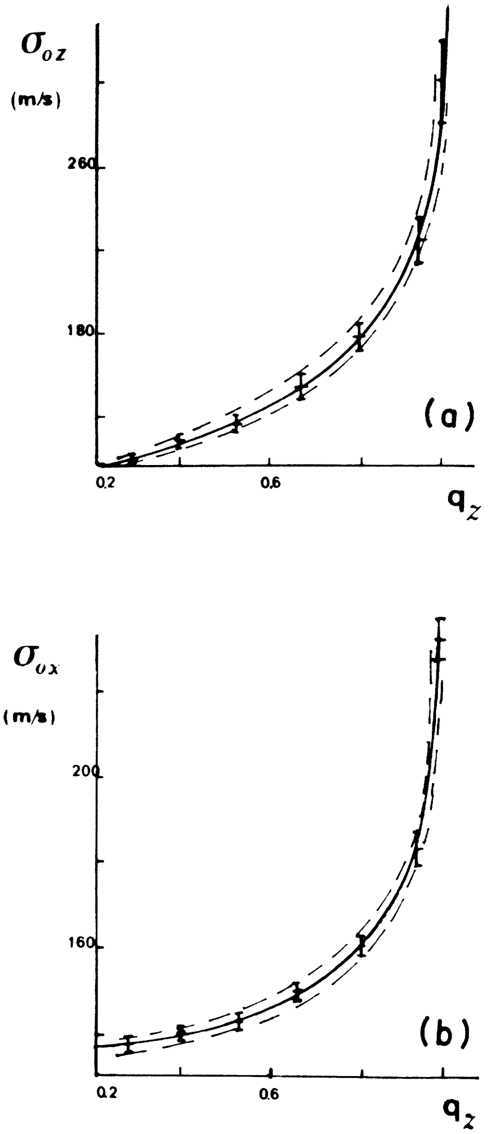

FIG. 3. Variation of the parameters (a) σ_{0z} and (b) σ_{0x} of the distribution law of the ions in the case of a Gaussian pattern (3D model), along the isobeta $\beta_z = 0.2$.

buffer gas is considered to be in a Maxwellian equilibrium at a temperature of 300 K with a density such that the assumption of the rarity of collision holds (see Sec. I). These are treated according to a classical hard-sphere model. The integral of (2.8) is calculated Monte Carlo fashion. By using a variance reduction technique, it is possible to obtain a precision of approximately 1% with 10000 samples. Under these conditions, each evaluation of the integral needs ten seconds of CDC-750 computer time. The parameters of f_0 are studied for different points (a,q) in the stability diagram and for several buffer gases. Note that σ_{0z} and σ_{0x} are independant of Ω.

A. Computations of σ_{0z} and σ_{0x} and suitability of the Gaussian approximation

1. Helium

We calculate σ_{0z} and σ_{0x} for 26 points of the stability diagram. Along the axis $a = 0$, the Gaussian model is entirely valid from criterions described above since c is near to 0.95($\pm$0.05). When we move the working point (a,q) in the stability diagram, the component upon $\vec{Oz}$ loses this quality when β_x becomes greater than 0.4 or 0.5 Figure 3 shows the variation of σ_{0z} and σ_{0x} along an isobeta. With the help of similar curves obtained for various isobeta we represent points on the stability diagram corresponding to contours of σ_{0z} and σ_{0x} (Fig. 4). In a region near the origin these parameters are practically equal to 138 m/s (which is the magnitude of the Maxwell velocity of cesium atoms at the same temperature). When we go away from the origin, these parameters, chiefly σ_{0z}, increase.

2. Neon

In the domain of adiabatic approximation, σ_{0z} and σ_{0x} are slightly greater that the values obtained with helium ($\sigma_{0z} = 147 \pm 3$ m/s, $\sigma_{0x} = 147 \pm 3$ m/s), f_0 stays Gaussian in a region placed on the left of a line passing approximately through the points ($a = 0, q = 0.6$) and ($\beta_z = 0.2, \beta_r = 0.2$). σ_{0z} and σ_{0x} are then, respectively, near 170 and 160 m/s.

3. Argon

With this buffer gas, f_0 is Gaussian only in a little region close to origin. In this case, σ_{0z} lies between 161 to 178 m/s and σ_{0x} varies in the range of 162 to 172 m/s.

4. Krypton

Here, results never allow one to suppose that the distribution of ions is Gaussian, even for points very near to the origin ($a = 0$, $q = 0.05$ for instance).

B. Physical parameters

For a better understanding of these results we calculate spatial dispersions and ionic temperatures

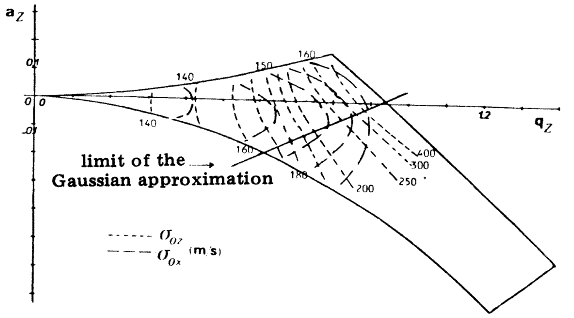

FIG. 4. Variation of the parameters σ_{0z} and σ_{0x} of the distribution law of the ions in the case of Gaussian pattern (3D model) in the stability diagram. (The uncertainty can be found from the envelope of the curves represented in Fig. 3.) The buffer gas is helium.

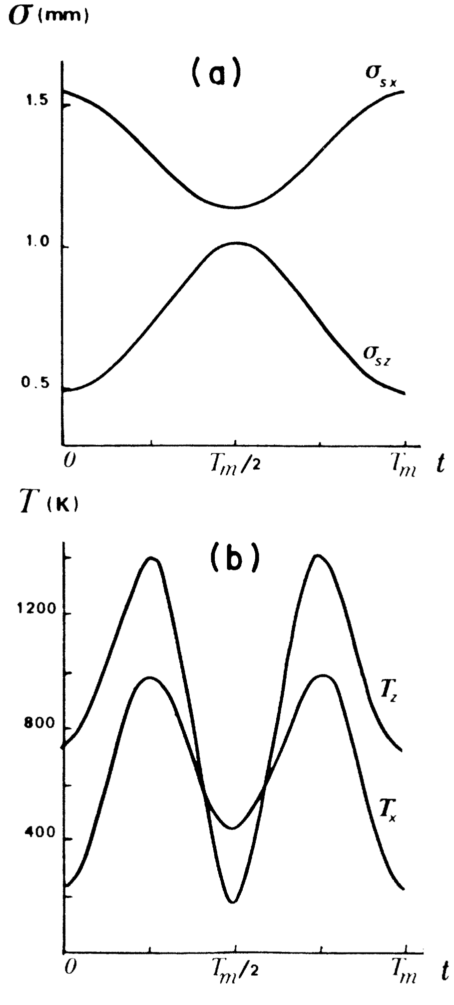

FIG. 5. (a) Temporal variation of the spatial dispersion $\sigma_{sz}(t)$,$\sigma_{sx}(t)$ and (b) of the pseudotemperatures $T_z(t)$ and $T_x(t)$ of the stored population.

with the formulas (3.4)–(3.7). This illustration of the previous section is made only in the case of helium.

Within the frame of adiabatic approximation, the temporal variations of the statistical parameters can be easily estimated with approximate relations such as

$$\sigma_{sz}(t)=\sigma_{0z}\left|1-\frac{q_z}{2}\cos\Omega t\right| \Big/ \omega_x \ ,$$

$$T_z(t)\simeq\frac{m}{k}\sigma_{0z}^2(1+2\sin^2\Omega t) \ .$$

In this case $\omega_x\simeq\omega_z/2$ and $\sigma_{0x}\simeq\sigma_{0z}$, then $\sigma_{sx}(t)\simeq2\bar{\sigma}_{sz}(t)$ and $T_x(t)\simeq T_z(t)$.

Outside this domain, it is difficult to foresee the magnitude and the shape of these variations. In Fig. 5 we represent $\sigma_{sz}(t)$, $\sigma_{sx}(t)$, $T_z(t)$, and $T_x(t)$ computed for a given working point. Actually, the shape of this curve varies very little in the stability diagram. $\sigma_{sz}(t)$ and $\sigma_{sx}(t)$ oscillate once during the period T_m and are in opposite phase. $T_z(t)$ and $T_x(t)$ oscillate twice during the same duration and are almost in phase. The relative amplitudes of $\sigma_{sz}(t)$ and $\sigma_{sx}(t)$ are of the order of q, those of $T_z(t)$ and $T_x(t)$ are near 3 and 2, respectively. In the region where f_0 is quasi-Gaussian, the minimal values of $T_z(t)$ and $T_x(t)$ are always approximately equal to 180 and 220 K, respectively. The maximums depend on the working point and can reach 12 000 and 10 000 K for each one.

The average values are drawn in Fig. 6. Note that $\bar{\sigma}_{sz}$ and $\bar{\sigma}_{sx}$ are strongly dependant on the driving frequency (since $\omega\simeq\beta\Omega/2$). The contour line of $\bar{\sigma}_{sz}$ (respectively, $\bar{\sigma}_{sx}$) roughly follows the isobeta β_z (respectively, β_r) except when the Mathieu coefficients vary in the opposite direction of the fundamental frequency, i.e., when a_z is positive (respec-

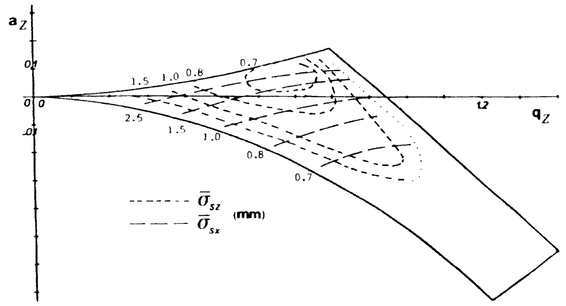

FIG. 6. Variation of the temporal average of the spatial dispersions $\bar{\sigma}_{sz}$ and $\bar{\sigma}_{sx}$ of the stored population in the stability diagram when the buffer gas is helium.

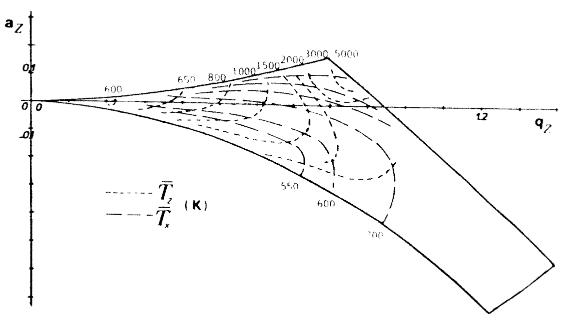

FIG. 7. Variation of the temperatures $\overline{T}_z$ and $\overline{T}_x$ of the stored population in the stability diagram when the buffer gas is helium.

tively, a_x) and the absolute value of q is sufficiently great. These parameters must be infinite when $\beta_z \simeq 0$ (respectively, $\beta_r \simeq 0$), i.e., when the confinement is null. Therefore, they must increase strongly when one approaches these boundaries as can be seen in Fig. 6. Figure 7 shows the contour lines corresponding to the temperature $\overline{T}_z$ and $\overline{T}_x$. These temperatures also reach great values for regions near the limits. For a given working point the temperature following x is less great than that following z, except near the isobeta $\beta_r = 0.1$. Generally, $\overline{T}_x$ varies less than $\overline{T}_z$.

These results allow us to specify the optimal working conditions. For instance, the space charge, all things being equal, increases when the spatial dispersions decrease. It seems well advised to choose a working point where spatial dispersions are not very small. On the other hand, we can see that the ionic temperatures are smaller near the axis $a=0$ and for $q \lesssim 0.4$. In this case, $T_x(t)$ is practically smaller than $T_z(t)$ and it can be useful to know this for optical measurements, for instance.

The values of these parameters are smaller than the experimental ones.[26,27] Several reasons can explain this difference. Space charge tends to heat the ions. Collisions with heavy ions are possible. Defects of the trap device also increase the ionic temperatures. Moreover, the experimental depth of the confinement was weaker than the theoretical one and measurements could be done before the asymptotic regime was reached.

VI. CONCLUSION

We have presented a method based upon a realistic model (3D model) which permits us to find the form of the spatial and energy distributions and to evaluate their parameters when the distributions are Gaussian. We have shown how the properties of these distributions evolve within the stability diagram. Qualitatively these results corroborate another previously obtained by the authors[13,22] with approximate models. However, the quantitative differences show the need of the present study. We delimited the regions where the ionic density is quasi-Gaussian according to the buffer gas and computed the statistic parameters with reasonable accuracy.

This method can be extended for non-Gaussian repartition by generalizing the 3D model with several parameters.

This work was done by neglecting space charge (number of ions being of the order of 10^4). However, it is also interesting for the study of nondilute confined population. Actually we have established, on the other hand, a formalism which permits one to evaluate the space-charge effect and for which it is necessary to know the energy and spatial parameters in absence of space charge.[24] With this formalism, it is possible to take account of these collective phenomena when f_0 is Gaussian (the evaluation of the disturbing term in the motion equation being too long in the opposite case to be in our model). Therefore, the present estimate of the parameters will allow us to systematically study the characteristics of the movement[25] in presence of weak space charge and to check that some properties of the motion remain realistic when the number of ions is increased. If this is so, it will be possible to know the energy and spatial properties, particularly the form of the distribution and to calculate the spatial dispersion and the ionic temperature in the whole stability diagram without neglecting the space charge.

ACKNOWLEDGMENT

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APPENDIX

Let $s_0 = (\omega_x x_0)/[1+A_x(0)]$ and $s_0 = \dot{x}_0/[1+D_x(0)]$; t_0 and t_0 are the corresponding values for z_0 and $\dot{z}_0$ and let $\gamma(s_0,\dot{s}_0,t_0,t_0)$ be the representation of a function $g(\vec{x}_0,\dot{\vec{x}}_0)$. Setting

$$f_0(x_0(s_0),\dot{x}_0(\dot{s}_0),0,0,z_0(t_0),\dot{z}_0(\dot{t}_0)) = \varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)$$

(2.4) allow us to write

$$\int \gamma(s_0,\dot{s}_0,t_0,\dot{t}_0)\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)ds_0 d\dot{s}_0 dt_0 d\dot{t}_0 = \int \gamma(s_k,\dot{s}_k,t_k,\dot{t}_k)\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)ds_0 d\dot{s}_0 dt_0 d\dot{t}_0 \; .$$

Choosing a function γ such as

$$\gamma(s_0,\dot{s}_0,t_0,\dot{t}_0)=\exp\left[i(\lambda_0,\lambda_0')\begin{bmatrix}s_0\\ \dot{s}_0\end{bmatrix}\right],$$

then

$$\int\exp\left[i(\lambda_0,\lambda_0')\begin{bmatrix}s_0\\ \dot{s}_0\end{bmatrix}\right]\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)ds_0d\dot{s}_0dt_0d\dot{t}_0$$
$$=\int\exp\left[i(\lambda_0,\lambda_0')\begin{bmatrix}s_k\\ \dot{s}_k\end{bmatrix}\right]\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)$$
$$\times ds_0d\dot{s}_0dt_0d\dot{t}_0\,. \qquad \text{(A1)}$$

From (2.6) the vector $\binom{s_k}{\dot{s}_k}$ is deduced from $\binom{s_0}{\dot{s}_0}$ by a rotation of the angle $\omega_x kT_m$:$\mathscr{R}(\omega_x kT_m)$ and (A1) become

$$\int\exp\left[i(\lambda_0,\lambda_0')\begin{bmatrix}s_0\\ \dot{s}_0\end{bmatrix}\right]\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)ds_0d\dot{s}_0dt_0d\dot{t}_0$$
$$=\int\exp\left[i(\lambda_0,\lambda_0')\mathscr{R}(\omega_x kT_m)\begin{bmatrix}s_0\\ \dot{s}_0\end{bmatrix}\right]$$
$$\times\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)ds_0d\dot{s}_0dt_0d\dot{t}_0$$

which implies that the Fourier transform of this relation is given by

$$\hat{\varphi}(\lambda_0,\lambda_0')=\hat{\varphi}(\lambda_1,\lambda_1')\,,$$

where λ_1 and λ_1' are obtained from λ_0 and λ_0' by a rotation of the angle $-\omega_x kT_m$. Since $\omega_x T_m$ is an irrational number, this means that $\hat{\varphi}$ is isotropic, i.e., $\hat{\varphi}$ is function of $(\lambda_0^2+\lambda_0'^2)^{1/2}$. Therefore, $\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)$ is also isotropic and

$$\varphi(s_0,\dot{s}_0,t_0,\dot{t}_0)=\varphi_1((s_0^2+\dot{s}_0^2)^{1/2},t_0,\dot{t}_0)\,.$$

The same considerations are applied to φ_1, for a function γ depending on t_0 and $\dot{t}_0$, to give

$$\varphi_1((s_0^2+\dot{s}_0^2)^{1/2},t_0,\dot{t}_0)=\varphi_2((s_0^2+\dot{s}_0^2)^{1/2},(t_0^2+\dot{t}_0^2)^{1/2})$$

and finally, from (2.7),

$$\varphi_2((s_0^2+\dot{s}_0^2)^{1/2},(t_0^2+\dot{t}_0^2)^{1/2})=\psi(u_x,u_z)\,.$$

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