Ideal Gas Approximation for an Ion Cloud in a Penning Trap

Martin Kretzschmar

Institut für Physik, Johannes-Gutenberg-Universität, Mainz, West-Germany

Z. Naturforsch. **45a**, 979–985 (1990); received May 21, 1990

Assuming a sufficiently low density of the trapped particles the methods of equilibrium statistical mechanics for non-interacting particles are used to find expectation values and distribution functions for the most interesting 1-particle observables. The results are applied in a perturbation calculation to estimate space charge effects at low particle densities.

1. Introduction

Penning traps are very useful experimental devices wherever high precision measurements require spatial confinement of charged particles over prolonged periods of time. (For general reviews see [1] and [2].) Some experiments are done with single (or very few) particles, but usually one has to deal with a low density cloud of charged particles containing on the order of 10^2 to 10^4 particles. The analysis of a specific experiment requires understanding not only of the individual particle orbits [3], but also of the collective properties of the particle cloud. One expects that over a period of time a state of equilibrium is attained, which can be studied using standard methods of statistical physics [4]. For a low density cloud it seems reasonable to assume that the particles move mainly independently of each other, except for occasional close encounters and the mutual Coulomb repulsion of the particles. On the one hand, by causing an exchange of energy, momentum and angular momentum between the particles, these interactions are instrumental in establishing a thermal equilibrium in the particle cloud, on the other hand, they may be considered as only a negligible perturbation to the average particle motion, provided the time average of the interaction potentials is small compared to the average energy of a single charged particle. For particle densities which are low enough for these assumptions to hold, one may attempt a description of the particle cloud as an ideal gas of non-interacting particles in thermal equilibrium. For reasons of simplicity we assume an ideal Penning trap (no anharmonic perturbations) and the absence of a background of neutral particles.

At a first glance, the use of standard methods of statistical physics seems to be precluded by the fact that the hamiltonian of a charged particle in a Penning trap is unbounded from below due to the magnetron motion. For the resolution of this difficulty it is important to observe that aside from the hamiltonian there exists another quantity of the type of an angular momentum* that is conserved by the single particle hamiltonian as well as by the two-particle interactions. Large amplitudes of the magnetron motion (i.e. large negative energies) require large values of this conserved quantity, therefore the additional conservation law stabilizes the magnetron motion of the trapped particles. A successful statistical approach must take proper account of this circumstance [5].

In the natural gauge for the magnetic vector potential the conserved quantity can be identified with the canonical angular momentum component corresponding to the direction of the magnetic field, so that this gauge provides a particularly convenient language. In the natural gauge it is thus justified to say that conservation of canonical angular momentum is the dominant factor in stabilizing the magnetron motion. For clarity let us emphasize that all probability distributions and expectation values of observable quantities are actually gauge independent.

2. Theoretical Framework

We consider the trapped particles as classical particles obeying Maxwell-Boltzmann statistics and

Reprint requests to Prof. Dr. M. Kretzschmar, Institut für Physik, Universität Mainz, P.O. Box 39 80, D-6500 Mainz.

* In cylindrical coordinates the conserved quantity is $mr^2(\dot{\varphi}+\frac{1}{2}\omega_c)$, where ω_c is the cyclotron frequency. This quantity is conserved irrespective of our choice of gauge for the magnetic vector potential.

0932-0784 / 90 / 0800-0979 $ 01.30/0. – Please order a reprint rather than making your own copy.

apply the method of the canonical ensemble. The particle number N is fixed, the total energy H^N and the total canonical angular momentum L^N (more precisely the component in the direction of the magnetic field) are treated as conserved quantities. The N-particle phase space Γ^N is parametrized by coordinates $X^N=(X_1, X_2, \ldots, X_N)$, where X_k denotes a set of 6 canonical coordinates (e.g. $\boldsymbol{q}_k, \boldsymbol{p}_k$) in the phase space Γ_k of the k-th particle. First we construct a probability distribution ϱ^N on the N-particle phase space with the property that the entropy

$$S=-k_{\mathrm{B}} \int_{\Gamma^N} \mathrm{d}X^N \cdot \varrho^N \ln(h^{3N} \varrho^N) \tag{2.1}$$

assumes its maximum value (k_{B} and h denote Boltzmann's and Planck's constant respectively).

In addition we have subsidiary conditions for the probability density and the conserved quantities H^N, L^N:

$$\begin{aligned} 1 &= \int_{\Gamma^N} \mathrm{d}X^N \cdot \varrho^N, \\ \langle H^N \rangle &= \int_{\Gamma^N} \mathrm{d}X^N \cdot \varrho^N H^N = E, \\ \langle L^N \rangle &= \int_{\Gamma^N} \mathrm{d}X^N \cdot \varrho^N L^N = L, \end{aligned} \tag{2.2}$$

where E and L are the expectation values of the total energy H^N and the total canonical angular momentum L^N of the particle cloud. Following standard prescriptions of statistical physics (see Chapt. 9 in [4]) this is achieved by solving the variational problem

$$\begin{aligned} 0=\int_{\Gamma^N} \mathrm{d}X^N \cdot \delta\,[\alpha_0 \varrho^N + \beta \varrho^N (H^N+\alpha_L L^N) \\ -k_{\mathrm{B}} \varrho^N \ln(h^{3N} \varrho^N)], \end{aligned} \tag{2.3}$$

where the constants α_0, β, $\beta\alpha_L$ are Lagrange multipliers. The resulting condition

$$\alpha_0 - k_{\mathrm{B}} + \beta(H^N + \alpha_L L^N) - k_{\mathrm{B}} \ln(h^{3N} \varrho^N) = 0 \tag{2.4}$$

is solved for ϱ^N and yields the probability density

$$\varrho^N(X^N) = (h^{3N} Z_N)^{-1} \exp(-\beta[H^N + \alpha_L L^N]) \tag{2.5}$$

and the partition sum

$$Z_N = h^{-3N} \int_{\Gamma^N} \mathrm{d}X^N \exp(-\beta[H^N + \alpha_L L^N]). \tag{2.6}$$

When (2.4) is then multiplied by ϱ^N and integrated over Γ^N, comparison with the thermodynamic relation defining the free energy $F=U-S\cdot T$ leads to the identification

$$\beta = \frac{1}{k_{\mathrm{B}} T} \tag{2.7}$$

and to the definitions of the free energy F

$$F = -k_{\mathrm{B}} T \ln Z_N \tag{2.8}$$

and the inner energy U

$$U = E + \alpha_L \cdot L = -\frac{\partial}{\partial \beta} \ln Z_N. \tag{2.9}$$

It remains to determine the parameter α_L. To this end the partition sum is explicitly evaluated, assuming that the particles have no mutual interaction (ideal gas approximation) and that the total hamiltonian and angular momentum are the sums of the corresponding 1-particle quantities

$$H^N(X^N) = \sum_{k=1}^{N} H(X_k), \quad L^N(X^N) = \sum_{k=1}^{N} L(X_k), \tag{2.10}$$

Using a reference frame rotating with angular velocity Ω around the direction of the magnetic field (z-direction) and introducing cylindrical coordinates r, φ, z and their canonically conjugate momenta p_r, $p_\varphi = L$, p_z, the single particle hamiltonian can be written in the form [3]

$$\begin{aligned} H(X;\Omega) = \frac{p_r^2}{2m} + \frac{p_\varphi^2}{2mr^2} + \frac{p_z^2}{2m} + \frac{m}{2}\left(\frac{\omega_1}{2}\right)^2 r^2 \\ + \frac{m}{2}\omega_z^2 z^2 - \left(\frac{\omega_c}{2} + \Omega\right) p_\varphi. \end{aligned} \tag{2.11}$$

Here $\omega_c = qB/(mc)$ denotes the cyclotron frequency, ω_z the axial frequency, and ω_1 is defined by $\omega_1 = (\omega_c^2 - 2\omega_z^2)^{1/2}$.

The partition sum Z_N can now be explicitly calculated as $Z_N = (Z)^N$, where Z is the 1-particle partition sum

$$Z = h^{-3} \int_{\Gamma} \mathrm{d}X \cdot \exp(-\beta[H(X) + \alpha_L L(X)]). \tag{2.12}$$

Inserting (2.11) and $L(X) = p_\varphi$ and performing the integrations over r, φ, z, p_r, and p_z one obtains

$$\begin{aligned} Z = (\beta^2 \hbar\omega_z \hbar\omega_1)^{-1} \\ \cdot \frac{1}{\hbar} \int_{-\infty}^{+\infty} \mathrm{d}p_\varphi \exp\left(-\beta \frac{\omega_1}{2} |p_\varphi| - \beta\left(\alpha_L - \frac{\omega_c}{2} - \Omega\right) p_\varphi\right). \end{aligned} \tag{2.13}$$

A necessary and sufficient condition for the convergence of this integral is $(\omega_1/2) > |\alpha_L - (\omega_c/2) - \Omega|$. Replacing α_L by a new parameter λ, this condition can be expressed as $|\lambda|<1$ with

$$\lambda \frac{\omega_1}{2} = \alpha_L - \frac{\omega_c}{2} - \Omega \tag{2.14}$$

The integration in (2.13) can now be completed and yields

$$Z_N(\beta, \lambda) = [Z(\beta, \lambda)]^N = \left[\beta^3 \hbar \omega_z \left(\hbar \frac{\omega_1}{2}\right)^2 (1-\lambda^2)\right]^{-N}. \tag{2.15}$$

This result gives us immediate access to thermodynamic functions and expectation values that are of interest to us.

Free energy:

$$F = -\frac{1}{\beta} \ln Z_N = N k_B T \ln \left[\beta^3 \hbar \omega_z \left(\hbar \frac{\omega_1}{2}\right)^2 (1-\lambda^2)\right]. \tag{2.16}$$

Inner energy:

$$U = -\frac{\partial}{\partial \beta} \ln Z_N = \frac{3N}{\beta} = 3N k_B T. \tag{2.17}$$

Entropy:

$$S = \frac{1}{T}(U-F) = N k_B \left(3 - \ln \left[\beta^3 \hbar \omega_z \left(\hbar \frac{\omega_1}{2}\right)^2 (1-\lambda^2)\right]\right). \tag{2.18}$$

Expectation value of the canonical angular momentum (cf. (2.2)):

$$L = \langle L^N \rangle = -\frac{2}{\beta \omega_1} \cdot \frac{\partial}{\partial \lambda} \ln Z_N = -\frac{N k_B T}{(\omega_1/2)} \cdot \frac{2\lambda}{1-\lambda^2}. \tag{2.19}$$

Expectation value of the total energy (cf. (2.2), (2.9), (2.14)):

$$E = \langle H^N \rangle = U - \alpha_L L$$

$$= N k_B T \left(3 + \frac{2\lambda}{1-\lambda^2} \cdot \frac{\omega_c + \lambda \omega_1 + 2\Omega}{\omega_1}\right). \tag{2.20}$$

Note that the inner energy depends only on the temperature as one would expect for an ideal gas. Once the temperature is known the state variable λ is fixed by the expectation value of the canonical angular momentum. The total energy E coincides with the inner energy U (i.e. the energy of disordered thermal motion) only for a special choice of the angular velocity Ω of the reference frame, according to (2.14) $\alpha_L = 0$ implies $\Omega = -\frac{1}{2}(\omega_c + \lambda \omega_1)$. Thus the equality $E = U$ can be satisfied only if the angular velocity Ω of the reference frame is in the interval $-\omega_+ < \Omega < -\omega_-$, where ω_+ and ω_- denote the modified cyclotron frequency and the magnetron frequency, respectively. In particular, in the laboratory frame the relation $E = U$ can never be satisfied. (For a general discussion of the role of canonical angular momentum in statistical physics see [6], especially § 10 and § 34.)

3. Single Particle Distribution Functions and Expectation Values

Once the N-particle probability distribution ϱ^N has been found, and the relation between the state variables β and λ and the expectation values of the total energy and total canonical angular momentum have been determined, it is an easy matter to evaluate all 1-particle distribution functions and expectation values that are of interest to us. After selecting one particle and integrating over the coordinates and momenta of the remaining ones, the 1-particle probability distribution is obtained as

$$\varrho(X) = \beta^3 \hbar \omega_z \left(\hbar \frac{\omega_1}{2}\right)^2 (1-\lambda^2) \tag{3.1}$$

$$\cdot h^{-3} \exp\left(-\beta \left[H(X) + \left(\frac{\omega_c}{2} + \lambda \frac{\omega_1}{2} + \Omega\right) L(X)\right]\right).$$

On comparison with (2.11) one recognizes that $\varrho(X)$ is actually independent of Ω. By integrating over any five of the variables $r, \varphi, z, p_r, p_\varphi, p_z$ we obtain a distribution over the remaining variable. For example

$$\varrho(p_r) = \sqrt{\frac{\beta}{2\pi m}} \cdot \exp\left(-\frac{\beta}{2m} p_r^2\right), \tag{3.2}$$

$$\varrho(p_z) = \sqrt{\frac{\beta}{2\pi m}} \cdot \exp\left(-\frac{\beta}{2m} p_z^2\right), \tag{3.3}$$

$$\varrho(p_\varphi) = \begin{cases} \frac{1}{4}\beta\omega_1(1-\lambda^2) \exp\left(-\beta(1+\lambda)\frac{\omega_1}{2} p_\varphi\right) & \text{for } p_\varphi > 0, \\ \frac{1}{4}\beta\omega_1(1-\lambda^2) \exp\left(-\beta(1-\lambda)\frac{\omega_1}{2} p_\varphi\right) & \text{for } p_\varphi < 0, \end{cases}$$

$$\varrho(r) = \beta m (1-\lambda^2) \left(\frac{\omega_1}{2}\right)^2$$

$$\cdot r \exp\left(-\frac{1}{2}\beta m (1-\lambda^2)\left(\frac{\omega_1}{2}\right)^2 r^2\right), \tag{3.5}$$

$$\varrho(z) = \sqrt{\frac{\beta m}{2\pi}} \omega_z \cdot \exp(-\tfrac{1}{2}\beta m \omega_z^2 z^2). \tag{3.6}$$

These distributions imply the following expectation values:

$$\left\langle \frac{p_r^2}{2m} \right\rangle = \left\langle \frac{p_z^2}{2m} \right\rangle = \left\langle \frac{m}{2}\,\omega_z^2 z^2 \right\rangle = \tfrac{1}{2} k_B T, \tag{3.7}$$

$$\langle r^2 \rangle = \frac{2k_B T}{m(1-\lambda^2)} \cdot \left(\frac{2}{\omega_1}\right)^2, \tag{3.8}$$

$$\langle p_\varphi \rangle = -\frac{k_B T}{(\omega_1/2)} \cdot \frac{2\lambda}{1-\lambda^2}. \tag{3.9}$$

Further results can be derived by using other sets of canonical coordinates. If one remembers that the Jacobian of a canonical transformation equals unity, then the transformation of the integrals is trivial and requires only a rewriting of $H(X)+\alpha_L L(X)$. A particularly useful set of coordinates are the action-angle variables. As shown in [3], the hamiltonian then takes the form

$$H = (\omega_+ + \Omega)\, J_+ + (\omega_- + \Omega)\, J_- + \omega_z J_z \tag{3.10}$$

with $0 \leqq J_+ < \infty$, $0 \leqq J_z < \infty$, and $-\infty < J_- \leqq 0$. The 1-particle probability density becomes after integration over the angles

$$\varrho(J_+, J_-, J_z) = \beta^3 \omega_z \left(\frac{\omega_1}{2}\right)^2 (1-\lambda^2) \tag{3.11}$$

$$\cdot \exp\left(-\beta\left[(1-\lambda)\frac{\omega_1}{2} J_+ - (1+\lambda)\frac{\omega_1}{2} J_- + \omega_z J_z\right]\right).$$

After two further integrations one obtains

$$\varrho(J_+) = \beta(1-\lambda) \cdot \frac{\omega_1}{2} \cdot \exp\left(-\beta(1-\lambda) \cdot \frac{\omega_1}{2} \cdot J_+\right), \tag{3.12}$$

$$\varrho(J_-) = \beta(1+\lambda) \cdot \frac{\omega_1}{2} \cdot \exp\left(-\beta(1+\lambda) \cdot \frac{\omega_1}{2} \cdot |J_-|\right), \tag{3.13}$$

$$\varrho(J_z) = \beta\omega_z \cdot \exp(-\beta\omega_z J_z). \tag{3.14}$$

Physically the action variables represent the squares of the amplitudes R_+, R_-, Z of the modified cyclotron motion, the magnetron motion and the axial motion, respectively [3]. The expectation values of these quantities are therefore of great interest.

$$\langle R_+^2 \rangle = \frac{2}{m\omega_1} \langle J_+ \rangle = \frac{k_B T}{m(1-\lambda)} \cdot \left(\frac{2}{\omega_1}\right)^2, \tag{3.15}$$

$$\langle R_-^2 \rangle = -\frac{2}{m\omega_1} \langle J_- \rangle = \frac{k_B T}{m(1+\lambda)} \cdot \left(\frac{2}{\omega_1}\right)^2, \tag{3.16}$$

$$\langle Z^2 \rangle = \frac{2}{m\omega_z} \langle J_z \rangle = \frac{2k_B T}{m\omega_z^2}, \tag{3.17}$$

The average energies per particle residing in the modified cyclotron, magnetron and axial motions are

$$E_+ = (\omega_+ + \Omega)\, \langle J_+ \rangle = \frac{k_B T}{1-\lambda} \cdot \frac{\omega_+ + \Omega}{(\omega_1/2)}, \tag{3.18}$$

$$E_- = (\omega_- + \Omega)\, \langle J_- \rangle = -\frac{k_B T}{1+\lambda} \cdot \frac{\omega_- + \Omega}{(\omega_1/2)}, \tag{3.19}$$

$$E_z = \omega_z \langle J_z \rangle = k_B T. \tag{3.20}$$

The values for the laboratory frame are obtained with $\Omega = 0$. Note that the magnetron energy can not be positive, unless Ω is nonvanishing and in the range $-\infty < \Omega < -\omega_-$. Equipartition of the energy to the three oscillator modes holds in the special rotating reference frame where $\Omega = -\frac{1}{2}(\omega_c + \lambda\omega_1)$. In this particular frame $E_+ = E_- = E_z = \frac{1}{3} E = \frac{1}{3} U$. In the laboratory frame, on the other hand, energy is always unequally distributed between the three modes with most of the energy residing in the cyclotron mode.

As a final remark we compute the expectation values for the kinetic energy E_{kin} and the kinetic angular momentum Λ in the laboratory frame. Using

$$E_{\text{kin}} = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$

$$= H_{\Omega=0} - \frac{m}{2}\,\omega_z^2 (z^2 - \tfrac{1}{2}(x^2+y^2)), \tag{3.21}$$

$$\Lambda = L - m\frac{\omega_c}{2}(x^2+y^2), \tag{3.22}$$

and (2.20), (3.7), and (3.8) we find

$$\langle E_{\text{kin}} \rangle = k_B T \cdot \left(\frac{1}{2} + \frac{(\omega_c + \lambda\omega_1)^2}{\omega_1^2 (1-\lambda^2)}\right), \tag{3.23}$$

$$\langle \Lambda \rangle = -\frac{k_B T}{1-\lambda^2} \cdot \left(\frac{2}{\omega_1}\right)^2 (\omega_c + \lambda\omega_1), \tag{3.24}$$

According to (3.7) a measurement of $\langle \dot{r}^2 \rangle$ and $\langle \dot{z}^2 \rangle$ by Doppler spectroscopy on trapped ions can serve as experimental determination of the temperature T.

4. Application to an Estimate of Space Charge Effects

The space charge distribution represented by a cloud of trapped charged particles causes shifts of the characteristic frequencies ω_+, ω_-, ω_z, and the originally sharp values of these frequencies become smeared into distributions of finite width. It is a problem of considerable practical importance to obtain estimates of these effects. Thermodynamic perturbation theory, § 32 in [6], is expected to yield reasonable results in physical situations where the number of trapped particles is sufficiently low, so that the energy of the mutual Coulomb repulsion represents only a small correction to the total energy of the particle cloud.

$$\left\langle \sum_{i<j} \frac{q^2}{|\boldsymbol{x}_i-\boldsymbol{x}_j|} \right\rangle = \tfrac{1}{2} N(N-1) \left\langle \frac{q^2}{|\boldsymbol{x}_1-\boldsymbol{x}_2|} \right\rangle \ll N k_B T \left(3 + \frac{2\lambda}{1-\lambda^2} \cdot \frac{\omega_c + \lambda\omega_1}{\omega_1}\right). \tag{4.1}$$

Each single particle feels on the average a perturbing potential $\delta\Phi(\boldsymbol{x})$ due to the other $N-1$ particles:

$$\delta\Phi(\boldsymbol{x}) = \tfrac{1}{2}(N-1) \int \mathrm{d}\boldsymbol{x}_1 \frac{q^2 \varrho(\boldsymbol{x}_1)}{|\boldsymbol{x}-\boldsymbol{x}_1|}, \tag{4.2}$$

where $\varrho(\boldsymbol{x}_1)$ is the probability distribution (3.1) written in cartesian coordinates. Since the trapped particles move mainly near the center of the trap (origin of coordinates) one may try to approximate $\delta\Phi$ by a power series in $r^2 = x^2 + y^2$ and z^2 including terms up to fourth power in the coordinates:

$$\delta\Phi(\boldsymbol{x}) = \delta\Phi^{(0)} + \delta\Phi^{(2)}(\boldsymbol{x}) + \delta\Phi^{(4)}(\boldsymbol{x}) + \dots \tag{4.3}$$

This is easily accomplished by expansion of the denominator in terms of spherical harmonics and subsequent integration.

In order to state the result in a transparent and convenient fashion we introduce the following abbreviations (assuming $\omega_z^2 < (1-\lambda^2)(\omega_1/2)^2$):

$$\delta\Phi_0 = \tfrac{1}{2}(N-1)\, q^2 \omega_z \sqrt{\frac{\beta m}{2\pi}} = \tfrac{1}{2}(N-1) \cdot \frac{q^2}{\sqrt{2\pi\langle z^2\rangle}}, \tag{4.4}$$

$$a^2 = \frac{\beta m}{2}(1-\lambda^2)\left(\frac{\omega_1}{2}\right)^2 = \frac{1}{\langle r^2\rangle}, \tag{4.5}$$

$$u = \left(1 - \frac{\omega_z^2}{(1-\lambda^2)(\omega_1/2)^2}\right)^{-1/2}. \tag{4.6}$$

The first quantity $\delta\Phi_0$ essentially describes the order of magnitude of the perturbing potential energy, the second quantity defines a characteristic length scale $a^{-1} = \sqrt{\langle r^2\rangle}$. The third parameter u measures the "sphericity" of the charge distribution, we have $1 < u < \infty$ for prolate charge distributions with the limiting cases $u = \infty$ for spherical and $u = 1$ for cylindrical charge distributions.

Furthermore, for $k = 0, 1, 2, \dots$ a sequence of real functions $l_k(x)$ is defined by

$$l_k(x) = \sum_{n=0}^{\infty} \frac{1}{(n+\frac{1}{2})(n+\frac{3}{2})\dots(n+k+\frac{1}{2})} \cdot \frac{1}{x^{2n}} = \sum_{n=0}^{\infty} \frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+k+\frac{3}{2})} \cdot \frac{1}{x^{2n}} \tag{4.7}$$

obeying the recursion relation

$$k \cdot l_k(x) = (1-x^2) \cdot l_{k-1}(x) + \frac{2^k x^2}{1 \cdot 3 \dots (2k-1)}. \tag{4.8}$$

These functions can also be written in a closed form. For the first three functions it reads

$$l_0(x) = x \cdot \ln\left(\frac{x+1}{x-1}\right), \tag{4.9}$$

$$l_1(x) = (1-x^2) \cdot l_0(x) + 2x^2, \tag{4.10}$$

$$l_2(x) = \tfrac{1}{2}(1-x^2)^2 \cdot l_0(x) + x^2(1-x^2) + \tfrac{2}{3}x^2. \tag{4.11}$$

From the series expansion and from the closed form one easily obtains the limiting values $l_0(1) = \infty$, $l_0(\infty) = 2$, $l_1(1) = 2$, $l_1(\infty) = \frac{4}{3}$, $l_2(1) = \frac{2}{3}$, $l_2(\infty) = \frac{8}{15}$.

The series expansion (4.3) can now be explicitly stated as follows:

$$\delta\Phi^{(0)} = \delta\Phi_0 \cdot l_0(u), \tag{4.12}$$

$$\delta\Phi^{(2)} = \delta\Phi_0 \cdot a^2 [z^2(l_1(u) - 2) - \tfrac{1}{2} r^2 l_1(u)], \tag{4.13}$$

$$\delta\Phi^{(4)} = \delta\Phi_0 \cdot a^4 \left[z^4 \left(l_2(u) - \frac{1}{3} - \frac{1}{3u^2} \right) - 3z^2 r^2 \left(l_2(u) - \frac{2}{3} \right) + \frac{3}{8} r^4 l_2(u) \right]. \tag{4.14}$$

This result is immediately accessible to physical interpretation. The constant term $\delta\Phi^{(0)}$ represents the potential energy due to Coulomb repulsion for a test particle located exactly at the center of the trap. It is obvious that this energy must be an upper limit for $\delta\Phi(\boldsymbol{x})$. In conjunction with (4.1) we thus obtain an estimate for the particle numbers N for which our perturbation approach is expected to yield reliable results:

$$N \ll \sqrt{\frac{2\pi(k_B T)^3}{mc^2(\hbar\omega_z)^2}} \cdot \left(3 + \frac{2\lambda(\omega_c + \lambda\omega_1)}{(1-\lambda^2)\,\omega_1}\right) \cdot \left(\frac{q^2}{\hbar c} \cdot \frac{u}{2} \ln \frac{u+1}{u-1}\right)^{-1}. \tag{4.15}$$

This inequality should be interpreted in the sense that N ought to be smaller than the right hand side by several orders of magnitude.

The quadratic term $\delta\Phi^{(2)}$ can be combined with the single particle hamiltonian H of (2.11) and then leads to a redefinition of the characteristic frequencies, as has been discussed in detail in [7]:

$$\omega_z^{(2)} = \omega_z \sqrt{1+\mu}\,, \quad \omega_1^{(2)} = \sqrt{\omega_1^2 - 2\omega_z^2 \varkappa}\,,$$

$$\omega_\pm^{(2)} = \tfrac{1}{2}(\omega_c \pm \omega_1^{(2)}) \tag{4.16}$$

with

$$\mu = \delta\Phi_0 \cdot \frac{2a^2}{m\omega_z^2} \cdot (l_1(u) - 2), \quad \varkappa = \delta\Phi_0 \cdot \frac{2a^2}{m\omega_z^2} \cdot l_1(u). \tag{4.17}$$

In most experiments one works with trap parameters such that $\omega_z \ll \omega_1$. Then $u \approx 1$ and $l_1(u) \approx 2$, so that the correction to the axial frequency ω_z is expected to be very small. The corrections to the modified cyclotron and magnetron frequencies $\delta\omega_\pm^{(2)} = \omega_\pm^{(2)} - \omega_\pm^{(0)}$ are given by (with $\omega_1 = \omega_1^{(0)}$, $\omega_z = \omega_z^{(0)}$)

$$\begin{aligned}\delta\omega_\pm^{(2)} &= \pm\tfrac{1}{2}\,\delta\omega_1^{(2)} = \pm(\omega_1^{(2)} - \omega_1^{(0)}) \approx \mp \frac{\omega_z^2}{2\omega_1}\varkappa \\ &\approx \mp \frac{(N-1)\, l_1(u)}{\sqrt{2\pi}\, m\omega_1 \langle r^2\rangle} \cdot \frac{q^2}{\sqrt{\langle z^2\rangle}} \\ &\approx \mp \frac{\omega_1}{8\sqrt{2\pi}} (N-1)(1-\lambda^2)\, l_1(u) \frac{q^2}{\hbar c} \cdot \frac{\hbar\,\omega_z}{k_B T} \cdot \sqrt{\frac{mc^2}{k_B T}}.\end{aligned} \tag{4.18}$$

This result is in qualitative agreement with the estimates by other authors [1, 8].

Finally the influence of the 4th order term $\delta\Phi^{(4)}$ can be discussed using the perturbation theory developed in [7]. To this end z^4, $z^2 r^2$, r^4 have to be replaced by their time average over the single particle orbits $\overline{z^4}$, $\overline{z^2 r^2}$, $\overline{r^4}$ in order to obtain $\overline{\delta\Phi^{(4)}}$ as a function of the action variables J_+, J_-, J_z. Using (4.12) and (4.13) of [7] we find

$$\begin{aligned}\overline{z^4} &= \frac{3J_z^2}{2m^2\omega_z^2}, \\ \overline{z^2 r^2} &= \frac{2J_z(J_+ - J_-)}{m^2\omega_z\omega_1}, \\ \overline{r^4} &= \frac{4}{m^2\omega_1^2}(J_+^2 + J_-^2 - 4J_+J_-).\end{aligned} \tag{4.19}$$

To 4th order the characteristic frequencies of a single particle orbit are obtained from (3.40) of [7] as follows:

$$\omega_+^{(4)} = \omega_+^{(2)} + \delta\Phi_0 \cdot 3a^4 \left[-\frac{2}{m^2\omega_z\omega_1} J_z(l_2(u) - \tfrac{2}{3}) + \frac{1}{m^2\omega_1^2}(J_+ - 2J_-)\, l_2(u)\right],$$

$$\omega_-^{(4)} = \omega_-^{(2)} + \delta\Phi_0 \cdot 3a^4 \left[+\frac{2}{m^2\omega_z\omega_1} J_z(l_2(u) - \tfrac{2}{3}) + \frac{1}{m^2\omega_1^2}(J_- - 2J_+)\, l_2(u)\right],$$

$$\omega_z^{(4)} = \omega_z^{(2)} + \delta\Phi_0 \cdot 3a^4 \left[\frac{J_z}{m^2\omega_z^2}\left(l_2(u) - \frac{1}{3} - \frac{1}{3u^2}\right) - \frac{2}{m^2\omega_z\omega_1}(J_+ - J_-)\left(l_2(u) - \frac{2}{3}\right)\right].$$

It is important to note that these expressions depend on the action variables J_+, J_-, J_z. Considering the whole particle cloud, the values of the action variables are distributed according to the thermal distributions of (3.12)–(3.14) with thermal averages as given by (3.15)–(3.17). This circumstance implies that in 4th order perturbation theory we do not obtain sharp values for the characteristic frequencies, but a distribution reflecting the thermal distribution of the action variables.

A comparison of the thermal averages of the 4th order corrections with the 2nd order terms reveals that the power series expansion of (4.3) is not yet very accurate for the range of arguments needed. However, because of the alternating character of the series we can be confident that our perturbation result approximates the true shifts of the characteristic frequencies within a factor of about 2. On the other hand, the line shape evaluated from the 4th order terms is probably only qualitatively correct and will be modified when further terms of the power series expansion are taken into account.

5. Concluding Remarks

We have considered a small number of charged particles confined in a Penning trap, forming a low density particle cloud. For reasons of simplicity we have assumed the absence of a neutral particle background and of anharmonic perturbations of the trap.

The particle orbits are then essentially those of single particles in an ideal trap. Taking conservation of canonical angular momentum properly into account, the particle cloud has been described as a thermal equilibrium state characterized by a temperature T and an angular momentum parameter λ. Distribution functions and expectation values for the most interesting 1-particle observables have been obtained for reference frames rotating with arbitrary angular velocity Ω. It is interesting to see that equipartition of the energy between the modified cyclotron mode, the magnetron mode and the axial mode holds only in one special rotating reference frame. The average energy in the magnetron mode is negative for $\Omega > -\omega_-$, especially for $\Omega = 0$ (laboratory frame). The results have been used in a perturbation calculation to estimate frequency shifts due to space charge effects. It is found that these effects are rather important. The calculation leads to an upper limit of the particle numbers for which the whole approach may be expected to be valid. A semiquantitative understanding (valid perhaps within a factor of 2) of the frequency shifts and a qualitative understanding of the line shape are obtained in the lowest order approximation. An improvement of these estimates seems in principle possible with increasing mathematical efforts.

[1] D. J. Wineland and W. M. Itano, Adv. Atomic Mol. Phys. **19,** 135 (1983).
[2] L. S. Brown and G. Gabrielse, Rev. Mod. Phys. **58,** 233 (1986).
[3] M. Kretzschmar, Particle Motion in a Penning Trap, preprint to be published.
[4] L. E. Reichl, A Modern Course in Statistical Physics, University of Texas Press, Austin 1980.
[5] In a different context this point has been emphasized also by: J. H. Malmberg and T. M. O'Neil, Phys. Rev. Letters **39,** 1333 (1977). – T. M. O'Neil and C. F. Driscoll, Phys. Fluids **22,** 266 (1979).
[6] L. D. Landau and E. M. Lifschitz, Lehrbuch der Theoretischen Physik, Vol. V (Statistische Physik, Teil 1), 5. Auflage, Akademie-Verlag, Berlin 1979.
[7] M. Kretzschmar, Z. Naturforsch. **45a,** 965 (1990).
[8] J. B. Jeffries, S. E. Barlow, and G. H. Dunn, Int. J. of Mass Spectrometry and Ion Processes **54,** 169 (1983).