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Explicit, analytical radio-frequency heating formulas for spherically symmetric nonneutral plasmas in a Paul trap

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A B S T R A C T

We present explicit, analytical heating formulas that predict the heating rates of spherical, one-component nonneutral plasmas stored in a Paul trap as a function of cloud size S, particle number N, and Paul-trap control parameter q in the low-temperature regime close to the cloud $\rightarrow$ crystal phase transition. We find excellent agreement between our analytical heating formulas and detailed, time-dependent molecular-dynamics simulations of the trapped plasmas. We also present the results of our numerical solutions of a temperature-dependent mean-field equation, which are consistent with our numerical simulations and our analytical results. This is the first time that analytical heating formulas are presented that predict heating rates with reasonable accuracy, uniformly for all S, N, and q. An analytical formula for the Coulomb logarithm in the weak-coupling regime is also presented.

1. Introduction

The Paul trap [1,2] has long secured its place as an indispensable tool in many fields of science with applications ranging from atomic clocks [3] and quantum computers [4–6] to mass spectrometry [7] and particle physics [8]. Given its long and successful history, it is surprising that the Paul trap still offers unsolved, fundamental physics problems. For instance, if $N \geq 2$ charged particles are simultaneously stored in a Paul trap, the kinetic energy of the particles increases in time, i.e., they exhibit the phenomenon of radio-frequency (rf) heating. Rf heating cannot be switched off. It is a basic physical process that necessarily accompanies the operation of the trap. Surprisingly, although the existence of rf heating has been known [9–11] and studied [12–16] for a long time, explicit heating formulas, capable of predicting rf heating rates, have so far not been available. This paper addresses this deficiency. In particular, focusing on trapped clouds of charged particles of the same sign of charge (known as one-component, nonneutral plasmas [17]), we present explicit, analytical heating formulas that predict the heating rates of spherical, one-component, nonneutral plasmas consisting of N charged particles as a function of cloud size S and Paul-trap parameter q [1,2,13].

We define rf heating as the cycle-averaged power extracted from the rf field of the trap. There are two situations of theoretical and experimental interest. (A) With the help of a cooling mechanism, such as buffer-gas cooling [9,18] or laser cooling [12,13], the plasma may be brought to a stationary state in which the size of the ion cloud stays constant, on average, over extended periods of time. (B) After the stationary state is reached, the cooling may be switched off. From this point on, due to the nonlinear nature of the particle-particle interactions in the plasma [12,13], the plasma cloud will absorb energy from the rf trapping field, heat up, and expand. As discussed in Sec. 3.4, the heating rates in situations (A) and (B) are different, since in situation (A) the rf field has to provide additional power to counteract the dissipative losses due to the micromotion [2] of the trapped particles. To keep the discussion focused, we concentrate in this Letter on situation (A).

This Letter is organized as follows. In Sec. 2 we present the basic equations that underlie our theory of rf heating. In Sec. 3 we present our analytical and numerical methods together with a detailed comparison between numerically and analytically computed rf heating rates. Excellent agreement between the results of our numerical simulation data and our analytical rf heating formulas is obtained. As pointed out in Sec. 3.4, our heating formulas may also be used to obtain an analytical expression for the Coulomb log-

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arithm of weakly coupled one-component nonneutral plasmas in the Paul trap. In Sec. 4 we discuss our results. We conclude our paper in Sec. 5. For the convenience of the reader we also provide an appendix, in which we convert our dimensionless quantities and results to standard SI units.

2. Theory

The starting point of our work is the following set of dimensionless equations of motion that describe the motion of N charged particles in a hyperbolic Paul trap [16]

$$\ddot{\vec{r}}_i+\gamma\dot{\vec{r}}_i+[a-2q\sin(2t)]\begin{pmatrix} x_i \\ y_i \\ -2z_i \end{pmatrix}=\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{\vec{r}_i-\vec{r}_j}{|\vec{r}_i-\vec{r}_j|^3},\quad i=1,\ldots,N. \tag{1}$$

Here $\vec{r}_i=(x_i,y_i,z_i)$ denotes the position vector of particle number i, γ is the damping constant, t is the time, and a and q are the two dimensionless control parameters of the Paul trap [1,2,13]. The solutions $\vec{r}_i(t)$ of (1) are best represented as a superposition of a slow, large-amplitude macromotion [2], $\vec{R}_i(t)=(X_i(t),Y_i(t),Z_i(t))$, and a fast, small-amplitude micromotion [2], $\vec{\xi}_i(t)$, i.e.,

$$\vec{r}_i(t)=\vec{R}_i(t)+\vec{\xi}_i(t), \tag{2}$$

where, to lowest order,

$$\vec{\xi}_i(t)=-\frac{q}{2}\sin(2t)\begin{pmatrix} X_i(t) \\ Y_i(t) \\ -2Z_i(t) \end{pmatrix}. \tag{3}$$

While (2) and (3) are approximations, meant to bring out the structure of the solutions of (1), our numerical simulations of (1) (see Sec. 3.1) are numerically exact. The damping constant γ in (1) plays a dual role. In our numerical simulations we use γ as a convenient way to achieve a spherical, stationary state in which rf heating balances the cooling induced by γ. As shown in [16], we may then use the equality between heating and cooling in the stationary state to compute the rf heating rate according to

$$H=\frac{dE}{dt}=2\gamma E_{\rm kin}, \tag{4}$$

where E is the total cycle-averaged energy of the plasma cloud and $E_{\rm kin}$ is its cycle-averaged kinetic energy [16]. Since in this paper we focus on spherical trapped plasma clouds, and since spherical clouds are obtained for the choice $a=q^2/2$ [2,13], we assume this setting of the parameter a for the remainder of this paper. Spherical clouds in the stationary state are conveniently characterized by their size,

$$S=\lim_{n\to\infty}\frac{1}{n}\sum_{k=1}^{n}\left[\sum_{i=1}^{N}\vec{r}_i^{\,2}(k\pi)\right]^{1/2}, \tag{5}$$

where $\vec{r}_i$ is evaluated at multiples of π, where, according to (3), the micromotion amplitude vanishes.

3. Methods and results

In this section we present our numerical and analytical methods for evaluating the heating rate $H=H(S,N,q)$. The numerical results obtained in Section 3.1 provide the target data sets to be matched by our analytical formulas developed in Sec. 3.2. This succeeds to an excellent degree of accuracy. In Sec. 3.3, we compare the results of our molecular-dynamics simulations with the solutions of a nonlinear mean-field equation. Excellent agreement between the rf heating rates obtained by these two qualitatively different numerical methods is obtained. This provides an independent check of our molecular-dynamics simulations.

3.1. Molecular dynamics simulations

Using a 5th-order Runge–Kutta method [19], we performed extensive molecular-dynamics simulations [20] of (1), extracting rf heating rates as discussed in [15] directly via computation of dE/dt according to (4) for $N=50$, 100, 200, and 500 particles and $q=0.10$, 0.15, 0.20, 0.25, 0.30, and 0.35. The resulting rf heating rates are shown as a function of cloud size S as the black data points in Fig. 1. While rf heating rates for $q=0.2$ were already computed and presented in [15], the data set displayed in Fig. 1, covering six different q values, is more extensive than the data set presented in [15]. We checked that the rf heating rates in the $q=0.20$ panel of Fig. 1 are consistent with the rf heating rates presented in [15]. Fig. 1 shows that the heating rates increase with decreasing cloud size until a critical cloud size, S_c, is reached (the left-most data point in Fig. 1 corresponds to S_c). From then on, for still smaller clouds, the heating rate decreases with decreasing cloud size, which causes a run-away effect that swiftly takes a sub-critical ($S<S_c$) cloud into the crystalline state. The non-monotonic shape of the heating curve responsible for stable ($S>S_c$) and unstable ($S<S_c$) clouds is illustrated in Fig. 15 in [13].

3.2. Analytical heating formulas

Defining the temperature

$$T=\frac{1}{3}\lim_{n\to\infty}\frac{1}{n}\sum_{k=1}^{n}\sum_{i=1}^{N}\dot{\vec{r}}_i^{\,2}(k\pi), \tag{6}$$

of a plasma cloud in the stationary state [16], the kinetic energy of the plasma cloud may be evaluated immediately on the basis of (2). The result is [16]

$$E_{\rm kin}=\frac{3N}{2}\left(1+\frac{q^2}{4}\right)T+\frac{1}{2}q^2S^2, \tag{7}$$

where we assumed that the micro- and macromotions are uncorrelated. Since, in the stationary state, γ determines the cloud size S, we may write $\gamma=\gamma(S,N,q)$. This way, if $\gamma(S,N,q)$ is known, we may use (4) and (7) to compute $H(S,N,q)$ analytically.

Our analytical formula for $\gamma(S,N,q)$ is based on the q and N scaling of the critical gamma, $\gamma_c(N,q)$, at which the transition to the crystal occurs [21]. In [21] we found that for a given q, γ_c scales like an iterated-log law in N. In order to reveal the q dependence of γ_c, we performed extensive additional molecular-dynamics simulations and established that

$$\gamma_c(N,q)=C(q)\ln[\ln(N)]-D(q), \tag{8}$$

where

$$C(q)=1.31\times q^{4.57},\quad D(q)=0.13\times q^{3.77}. \tag{9}$$

Additional molecular-dynamics simulations then allowed us to determine the complete scaling of $\gamma(S,N,q)$. We found

$$\gamma(S,N,q)=\gamma_c(N,q)\exp\left[-2q^{0.9}\left(\frac{S-S_c(N,q)}{\sqrt{S_c(N,q)}}\right)\right], \tag{10}$$

where $S_c(N,q)$ is the critical cloud size at $\gamma=\gamma_c$. Since S_c is very close to the size $S_{\rm crystal}(N,q)$ of the crystal, we write

$$S_c(N,q)=S_{\rm crystal}(N,q)+\sigma(N,q), \tag{11}$$

where [16]